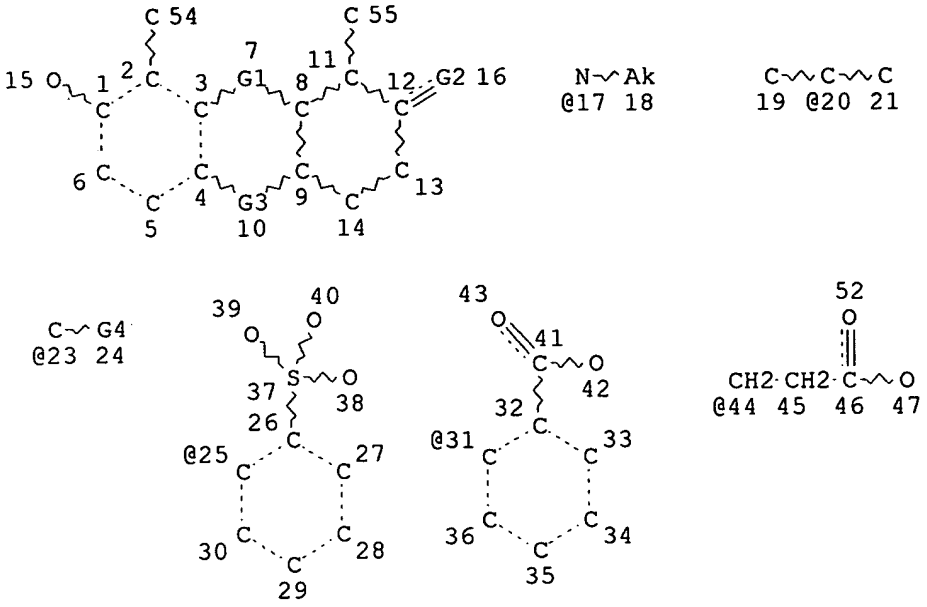
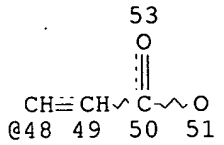
CA PLUS + CAOLD

=> d que
L46 STR



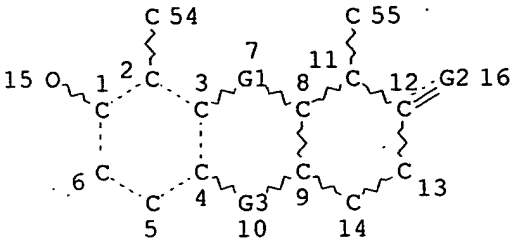


Considered. 07/08/03 MTC

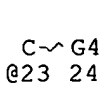
VAR G1=17/20/O/S/SE
VAR G2=O/S/SE
VAR G3=22/23
VAR G4=25/31/44/48
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 2
CONNECT IS E3 RC AT 11
CONNECT IS E2 RC AT 22
CONNECT IS E1 RC AT 38
CONNECT IS E1 RC AT 39
CONNECT IS E1 RC AT 40
CONNECT IS E1 RC AT 42
CONNECT IS E1 RC AT 47
CONNECT IS E1 RC AT 51
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

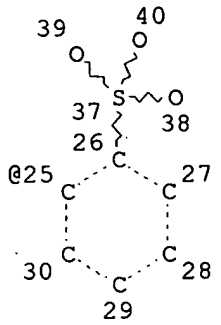
GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 55

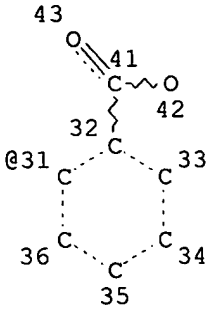
STEREO ATTRIBUTES: NONE
L48 93 SEA FILE=REGISTRY SSS FUL L46
L49 STR

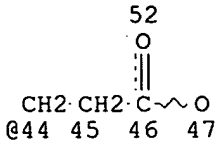


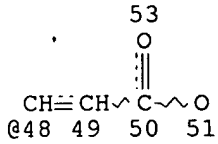
N @22











VAR G1=17/20/O/S/SE
VAR G2=O/S/SE
VAR G3=22/23
VAR G4=25/31/44/48
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 2
CONNECT IS E3 RC AT 11
CONNECT IS E2 RC AT 22
CONNECT IS E1 RC AT 38
CONNECT IS E1 RC AT 39
CONNECT IS E1 RC AT 40
CONNECT IS E1 RC AT 42
CONNECT IS E1 RC AT 47
CONNECT IS E1 RC AT 51
CONNECT IS M2 RC AT 54
CONNECT IS M2 RC AT 55
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 55

STEREO ATTRIBUTES: NONE
L50 2 SEA FILE=REGISTRY SUB=L48 SSS FUL L49
L51 2 SEA L50

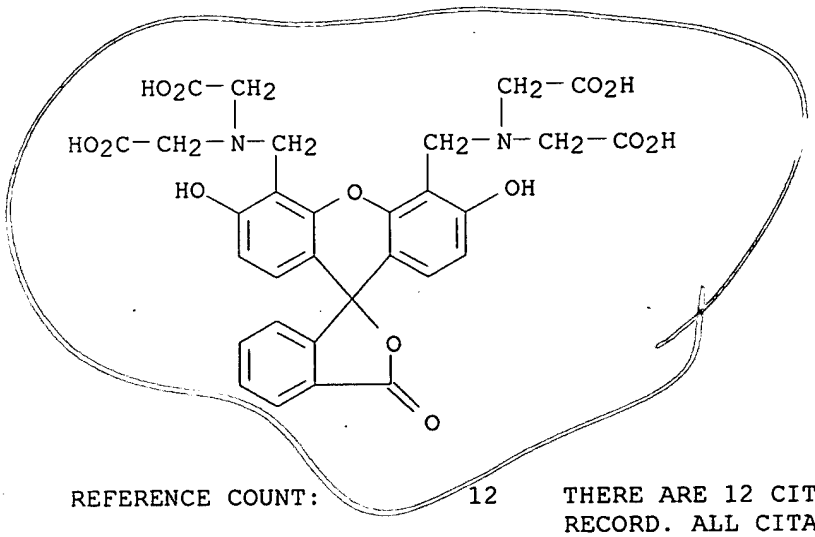
=> d ibib ab hitstr 1-2

L51 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:100905 HCAPLUS
DOCUMENT NUMBER: 132:228111
TITLE: Spectrofluorimetric study of the complexes between calcein and lanthanide(III) ions
AUTHOR(S): Berregi, Inaki; Del Campo, Gloria; Durand, J. Senen; Casado, J. Alfonso
CORPORATE SOURCE: Unit of Analytical Chemistry, Faculty of Chemistry, University of the Basque Country, San Sebastian, 20080, Spain
SOURCE: Analytical Letters (2000), 33(2), 277-295
CODEN: ANALBP; ISSN: 0003-2719
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The equil. of calcein, an H6L type fluorescent ligand, with lanthanide(III) ions, Ln(III), was studied spectrofluorometrically in aq. soln. at const. ionic strength .mu.=0.1 (KCl), pH 8.0 and 25.0.+-.0.1.degree.. Application of the mole ratio and continuous variation methods reveals the formation of 1:1 complexes. The conditional stability consts. (.beta.') were calcd. from the anal. of the obsd. fluorescence vs. [Ln(III)]/[calcein] mole ratio data by using an iterative nonlinear least-squares computer program. The values obtained for .beta.' are in the range 5.24 .times. 106-5.77 .times. 107. The thermodn. stability consts. (.beta.) were estd. by calcg. the side-reaction coeffs. (.alpha.) for lanthanides and calcein. The .beta. values obtained were 3.2 .times. 1012-3.6 .times. 1013.

IT **207124-64-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(calcein; complex formation between calcein and lanthanide(III) ions by spectrofluorimetry)

RN 207124-64-9 HCAPLUS
CN Glycine, N,N'-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)



see structure of EP 297,303 p. 4

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:511969 HCAPLUS
DOCUMENT NUMBER: 113:111969
TITLE: Enzyme-controlled-release system using a quinone-methide elimination reaction mechanism for use in immunoassays and pharmaceuticals
INVENTOR(S): Meneghini, Frank A.; Palumbo, Paul S.
PATENT ASSIGNEE(S): Polaroid Corp., USA
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9001558	A1	19900222	WO 1989-US1696	19890420
W: JP				
RW: DE, FR, GB, IT, NL				
US 5112739	A	19920512	US 1988-227141	19880802
EP 396642	A1	19901114	EP 1989-907960	19890420
EP 396642	B1	19940511		
R: DE, FR, GB, IT, NL				
JP 03500367	T2	19910131	JP 1989-507309	19890420
CA 1336586	A1	19950808	CA 1989-598563	19890503

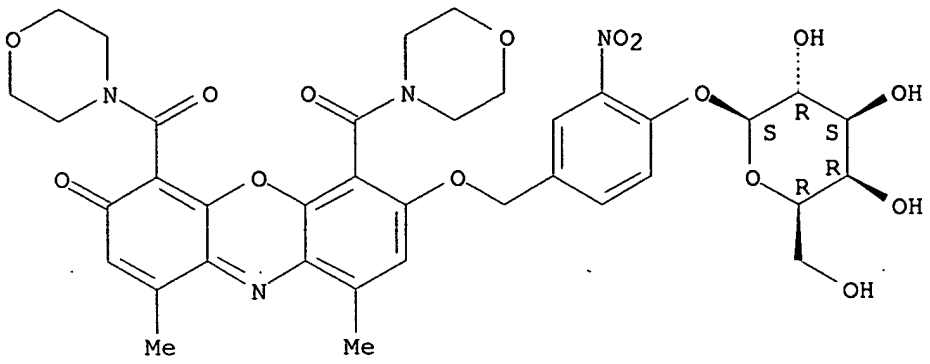
PRIORITY APPLN. INFO.: US 1988-227141 19880802
WO 1989-US1696 19890420

OTHER SOURCE(S): MARPAT 113:111969

AB An enzyme-controlled-release system uses compd. I (R, R1, R2, R3 = H, substituent affecting the mobility or reactivity of the compd., or a substituent including a biol. active group; X = leaving group and may be an org., organometallic, or inorg. moiety; Z = enzyme substrate cleavable by an active enzyme; CR2R3X is either ortho or para to the OZ moiety). An active enzyme cleaves the substrate, Z; the resultant active intermediate undergoes a quinone-methide elimination reaction to release the leaving group X. The system is useful for detecting an analyte of interest and may be used in, e.g., immunoassays, enzyme amplification systems, and the release of pharmacol. active ligands. (4-Resorufinylmethyl-2-nitrophenyl)-2,3,4,6-tetra-O-acetyl-.beta.-D-galactopyranoside was prepd. by heating a soln. of (4-chloromethyl-2-nitrophenyl)-2,3,4,6-tetra-O-acetyl-.beta.-D-galactopyranoside (prepn. given), Na resorufin, and a catalytic amt. of NaI in dry DMF at 70.degree. for 4 h. The galactosyl acetate protecting groups were removed with NaOMe. When the galactopyranoside was treated with .beta.-galactosidase, the leaving group release rate was 0.25 (compared with 1.0 for o-nitrophenolgalactoside).

IT **129046-75-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and dye controlled release from, by .beta.-galactosidase)
RN 129046-75-9 HCAPLUS
CN Morpholine, 4,4'-[[7-[[4-(.beta.-D-galactopyranosyloxy)-3-nitrophenyl]methoxy]-1,9-dimethyl-3-oxo-3H-phenoxazine-4,6-diyl]dicarbonyl]bis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


O
N
O
O
N
O
NO2
OH
O
R
OH
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R
O
R
OH
O
O
N
OH
Me
Me

Beilstein

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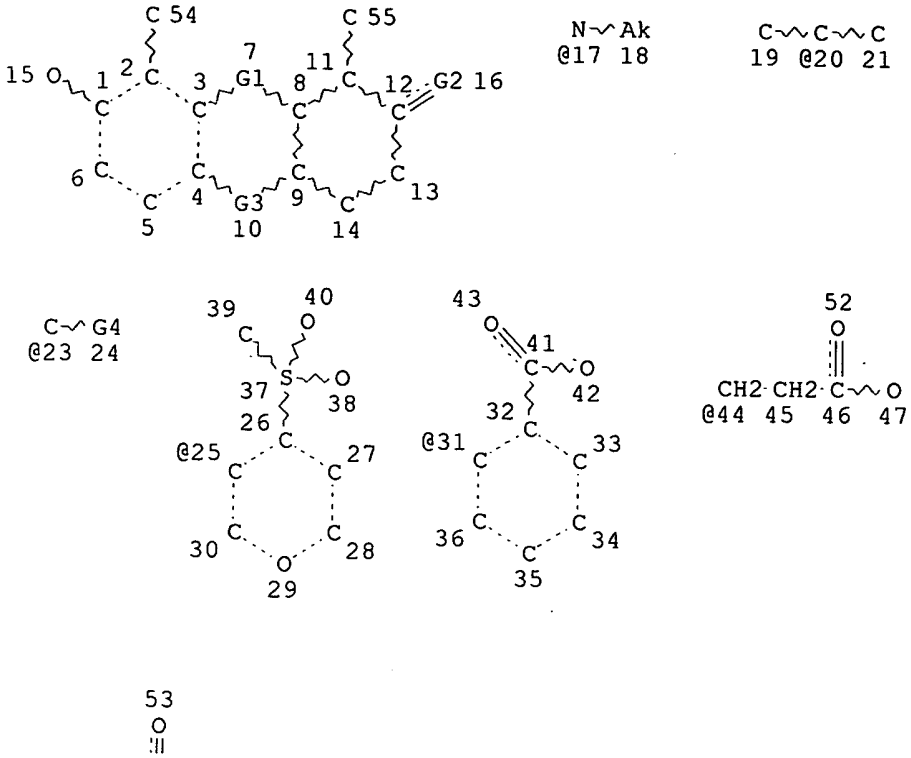
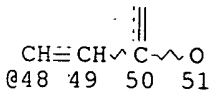
L18 STR



Considered
07/08/03
MEC

Page 1-A



Page 2-A
VAR G1=17/20/O/S/SE
VAR G2=O/S/SE
VAR G3=22/23
VAR G4=25/31/44/48
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 2
CONNECT IS E3 RC AT 11
CONNECT IS E2 RC AT 22
CONNECT IS E2 RC AT 27
CONNECT IS E2 RC AT 28
CONNECT IS E2 RC AT 29
CONNECT IS E2 RC AT 30
CONNECT IS E1 RC AT 38
CONNECT IS E1 RC AT 39
CONNECT IS E1 RC AT 40
CONNECT IS E1 RC AT 42
CONNECT IS E1 RC AT 47
CONNECT IS E1 RC AT 51

CONNECT IS M2 RC AT 54
CONNECT IS M2 RC AT 55
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

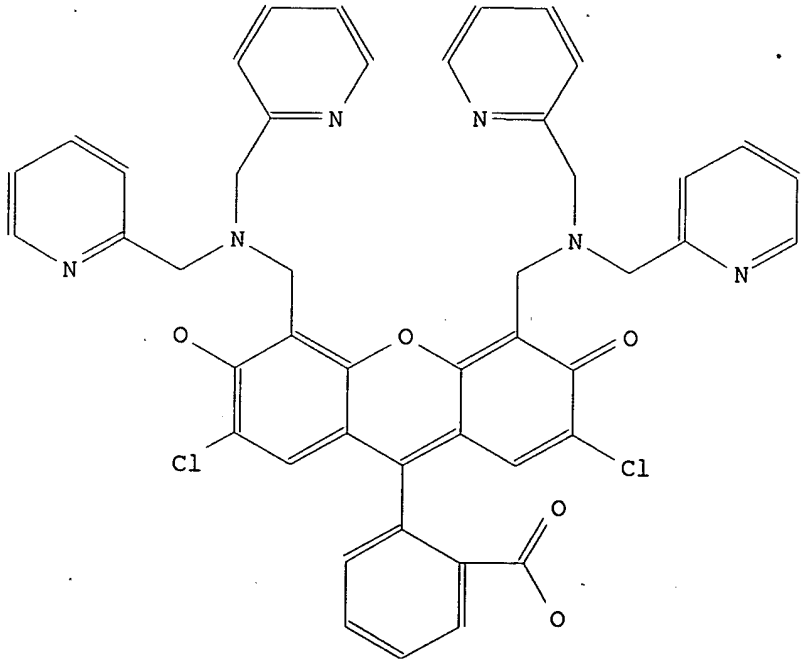
GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 55

STEREO ATTRIBUTES: NONE
L39 6 SEA FILE=BEILSTEIN SSS FUL L18

=> d l39 ide rx 1-6

L39 ANSWER 1 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	8749931
Chemical Name (CN):	2-<4,5-bis-<(bis-pyridin-2-ylmethyl-amino)-methyl>-2,7-dichloro-6-hydroxy-3-oxo-3H-xanthen-9-yl>-benzoic acid
Autonom Name (AUN):	2-<4,5-bis-<(bis-pyridin-2-ylmethyl-amino)-methyl>-2,7-dichloro-6-hydroxy-3-oxo-3H-xanthen-9-yl>-benzoic acid
Molec. Formula (MF):	C46 H36 Cl2 N6 O5
Molecular Weight (MW):	823.73
Lawson Number (LN):	27387, 20716
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7409990
Tautomer ID (TAUTID):	8237327
Entry Date (DED):	2001/04/26
Update Date (DUPD):	2001/04/26



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1

CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:
RX

Reaction ID (.ID):	8693040
Reactant BRN (.RBRN):	476398, 1270705, 1209228
Reactant (.RCT):	bis-pyridin-2-ylmethyl-amine, 2'.7'-Dichlor-fluorescein, formaldehyde
Product BRN (.PBRN):	8749931
Product (.PRO):	2-<4,5-bis-<(bis-pyridin-2-ylmethyl-amino)-methyl>-2,7-dichloro-6-hydroxy-3-oxo-3H-xanthen-9-yl>-benzoic acid
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8693040.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	46 percent (BRN=8749931)
Solvent (.SOL):	H2O, acetonitrile
Other Conditions (.COND):	Heating
Reaction Type (.TYP):	Condensation

Reference(s):

1. Walkup, Grant K.; Burdette, Shawn C.; Lippard, Stephen J.; Tsien, Roger Y., J.Amer.Chem.Soc., CODEN: JACSAT, 122(23), <2000>, 5644 - 5645; BABS-6267730

L39 ANSWER 2 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	382755
Chemical Name (CN):	1,7,9-triacetoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Autonom Name (AUN):	1,7,9-triacetoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Molec. Formula (MF):	C30 H29 N O16
Molecular Weight (MW):	659.56
Lawson Number (LN):	31516, 1155, 298
Compound Type (CTYPE):	heterocyclic

Constitution ID (CONSID):	364840
Tautomer ID (TAUTID):	383665
Beilstein Citation (BSO):	2-27-00-00396
Entry Date (DED):	1988/06/27
Update Date (DUPD):	1992/05/13

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
RSTR	Related Structure	1

L39 ANSWER 3 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	381789
Chemical Name (CN):	1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Autonom Name (AUN):	1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Molec. Formula (MF):	C27 H29 N O13
Molecular Weight (MW):	575.52
Lawson Number (LN):	31516, 298, 289
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	363470
Tautomer ID (TAUTID):	353176
Beilstein Citation (BSO):	2-27-00-00396
Entry Date (DED):	1988/06/27
Update Date (DUPD):	1992/05/13

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
CPD	Crystal Property Description	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

Reaction:
RX

Reaction ID (.ID): 5586134
Reactant BRN (.RBRN): 102415
Reactant (.RCT): 4.5.7-trioxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-tetraethyl ester, diazomethane
Product BRN (.PBRN): 381789
Product (.PRO): 1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX

Reaction RID (.RID): 5586134.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): diethyl ether
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX

Reaction ID (.ID): 5541629
Reactant BRN (.RBRN): 506007, 381789
Reactant (.RCT): zinc dust, acetic acid, 1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester

Product (.PRO): 2-oxy-4.5.7-trimethoxy-phenoxazine-tetracarboxylic acid-(1.3.6.8)-tetraethyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 5541629.1
Reaction Classification (.CL): Chemical behaviour (half reaction)
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX
Reaction ID (.ID): 545856
Reactant BRN (.RBRN): 381789
Reactant (.RCT): 1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Product BRN (.PBRN): 381797
Product (.PRO): 3-hydroxy-1,7,9-trimethoxy-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 545856.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): zinc dust, glacial acetic acid
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

L39 ANSWER 4 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 381658
Chemical Name (CN): 1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester-4-methyl ester
Autonom Name (AUN): 1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid 2,6,8-triethyl ester 4-methyl ester
Molec. Formula (MF): C26 H27 N O13
Molecular Weight (MW): 561.50
Lawson Number (LN): 31516, 298, 289
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 363139
Tautomer ID (TAUTID): 350886
Beilstein Citation (BSO): 2-27-00-00395
Entry Date (DED): 1988/06/27
Update Date (DUPD): 1992/05/13

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
CPD	Crystal Property Description	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Reaction:
RX

Reaction ID (.ID): 5586077
Reactant BRN (.RBRN): 102415
Reactant (.RCT): 4.5.7-trioxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-triethyl ester-(3.6.8), diazomethane
Product BRN (.PBRN): 381658
Product (.PRO): 1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester-4-methyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX

Reaction RID (.RID): 5586077.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): diethyl ether
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX

Reaction ID (.ID): 5586080
Reactant BRN (.RBRN): 506007, 381658

Reactant (.RCT): zinc dust, acetic acid, 1,7,9-trimethoxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester-4-methyl ester
Product BRN (.PBRN): 381663
Product (.PRO): 3-hydroxy-1,7,9-trimethoxy-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester-4-methyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX

Reaction RID (.RID): 5586080.1
Reaction Classification (.CL): Chemical behaviour
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

L39 ANSWER 5 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 380990
Chemical Name (CN): 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Autonom Name (AUN): 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Molec. Formula (MF): C24 H23 N O13
Molecular Weight (MW): 533.44
Lawson Number (LN): 31516, 298
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 363710
Tautomer ID (TAUTID): 370819
Beilstein Citation (BSO): 1-27-00-00386, 2-27-00-00395
Entry Date (DED): 1988/06/27
Update Date (DUPD): 1993/03/15

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1

BSO	Beilstein Citation	2
ED	Entry Date	1
UPD	Update Date	1
CPD	Crystal Property Description	1
MP	Melting Point	1
RSTR	Related Structure	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	10
RXREA	Substance is Reaction Reactant	6
RXPRO	Substance is Reaction Product	4

Reaction:
RX

Reaction ID (.ID):	545619
Reactant BRN (.RBRN):	381305
Reactant (.RCT):	1,3,7,9-tetrahydroxy-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Product BRN (.PBRN):	380990
Product (.PRO):	1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	545619.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	air
Note(s) (.COM):	Handbook

Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX

Reaction ID (.ID):	529039
Reactant BRN (.RBRN):	3526464
Reactant (.RCT):	2,4,6,2',4',6'-hexahydroxy-5,5'-imino-di-isophthalic acid tetraethyl ester
Product BRN (.PBRN):	381363, 380990
Product (.PRO):	6,8-dihydroxy-2-oxo-2H-benzo<b>cyclopent<e><1,4>oxazine-1,1,3,5,7-pentacarboxylic acid-1,3,5,7-tetraethyl ester, 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	529039.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	nitric acid
Note(s) (.COM):	Handbook

Reference(s):
1. Leuchs; Theodorescu, Chem.Ber., CODEN: CHBEAM, 43, <1910>, 1243

Reaction:
RX

Reaction ID (.ID):	529038
Reactant BRN (.RBRN):	3526464
Reactant (.RCT):	2,4,6,2',4',6'-hexahydroxy-5,5'-imino-di-isophthalic acid tetraethyl ester
Product BRN (.PBRN):	380990
Product (.PRO):	1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	529038.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	alcoholic ammonia
Note(s) (.COM):	Handbook

Reference(s):
1. Leuchs; Theodorescu, Chem.Ber., CODEN: CHBEAM, 43, <1910>, 1243

Reaction:
RX

Reaction ID (.ID):	504594
Reactant BRN (.RBRN):	3401756
Reactant (.RCT):	5-amino-2,4,6-trihydroxy-isophthalic acid diethyl ester
Product BRN (.PBRN):	380990
Product (.PRO):	1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	504594.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	alcohol
Note(s) (.COM):	Handbook

Reference(s):
1. Leuchs; Theodorescu, Chem.Ber., CODEN: CHBEAM, 43, <1910>, 1243

Reaction:
RX

Reaction ID (.ID):	5605735
Reactant BRN (.RBRN):	969212, 380990
Reactant (.RCT):	benzene, 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Product (.PRO):	4.5.7-trioxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-triethyl ester-(3.6.8)
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	5605735.1
Reaction Classification (.CL):	Chemical behaviour (half reaction)
Note(s) (.COM):	Handbook
Reference(s):	

1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX

Reaction ID (.ID):	5605733
Reactant BRN (.RBRN):	506104, 380990
Reactant (.RCT):	acetic acid ethyl ester, 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Product (.PRO):	4.5.7-trioxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-triethyl ester-(3.6.8)
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	5605733.1
Reaction Classification (.CL):	Chemical behaviour (half reaction)
Note(s) (.COM):	Handbook
Reference(s):	

1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX

Reaction ID (.ID):	5605721
Reactant BRN (.RBRN):	102415, 1696894, 380990
Reactant (.RCT):	diazomethane, diethyl ether, 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Product (.PRO):	4.5.7-trimethoxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-tetraethyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	5605721.1
Reaction Classification (.CL):	Chemical behaviour (half reaction)
Note(s) (.COM):	Handbook
Reference(s):	

1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX

Reaction ID (.ID):	5484062
Reactant BRN (.RBRN):	506007, 380990
Reactant (.RCT):	zinc dust, acetic acid, 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl

ester
Product (.PRO): 2.4.5.7-tetraoxy-phenoxazine-tetracarboxylic acid-(1.3.6.8)-tetraethyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 5484062.1
Reaction Classification (.CL): Chemical behaviour (half reaction)
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs; Theodorescu, Chem.Ber., CODEN: CHBEAM, 43, <1910>, 1243

Reaction:
RX
Reaction ID (.ID): 545434
Reactant BRN (.RBRN): 380990
Reactant (.RCT): 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Product BRN (.PBRN): 3157293
Product (.PRO): 4,6-dihydroxy-5-hydroxyimino-2-oxo-cyclohexa-3,6-diene-1,3-dicarboxylic acid diethyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 545434.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): aqueous-alcoholic alkaline solution, hydroxylamine
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs; Theodorescu, Chem.Ber., CODEN: CHBEAM, 43, <1910>, 1243
2. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 3

Reaction:
RX
Reaction ID (.ID): 545433
Reactant BRN (.RBRN): 380990
Reactant (.RCT): 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid tetraethyl ester
Product BRN (.PBRN): 3157293, 299769
Product (.PRO): 4,6-dihydroxy-5-hydroxyimino-2-oxo-cyclohexa-3,6-diene-1,3-dicarboxylic acid diethyl ester, 5-amino-2,4-dihydroxy-6-nitroso-isophthalic acid diethyl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 545433.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): alcohol, hydroxylamine

Note(s) (.COM): Handbook
Reference(s):
1. Leuchs; Theodorescu, Chem.Ber., CODEN: CHBEAM, 43, <1910>, 1243

L39 ANSWER 6 OF 6 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	380535
Chemical Name (CN):	1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester
Autonom Name (AUN):	1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid 2,6,8-triethyl ester
Molec. Formula (MF):	C22 H19 N O13
Molecular Weight (MW):	505.39
Lawson Number (LN):	31516, 298
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	363475
Tautomer ID (TAUTID):	367744
Beilstein Citation (BSO):	2-27-00-00395
Entry Date (DED):	1988/06/27
Update Date (DUPD):	1992/05/13

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	4
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	2

Reaction:

RX

Reaction ID (.ID):	5585509
Reactant (.RCT):	4.5.7-trioxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-tetraethyl ester
Product BRN (.PBRN):	380535
Product (.PRO):	1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester
No. of React. Details (.NVAR):	2

Reaction Details:

RX

Reaction RID (.RID):	5585509.1
Reaction Classification (.CL):	Preparation (half reaction)
Reagent (.RGT):	benzene
Note(s) (.COM):	Handbook
Reference(s):	

1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

RX

Reaction RID (.RID):	5585509.2
Reaction Classification (.CL):	Preparation (half reaction)
Reagent (.RGT):	acetic acid ester
Note(s) (.COM):	Handbook
Reference(s):	

1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:

RX

Reaction ID (.ID):	5585508
Reactant (.RCT):	4.5.7-trioxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-tetraethyl ester-N oxide
Product BRN (.PBRN):	380535
Product (.PRO):	1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester
No. of React. Details (.NVAR):	2

Reaction Details:

RX

Reaction RID (.RID):	5585508.1
Reaction Classification (.CL):	Preparation (half reaction)
Reagent (.RGT):	benzene
Note(s) (.COM):	Handbook
Reference(s):	

1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

RX

Reaction RID (.RID):	5585508.2
Reaction Classification (.CL):	Preparation (half reaction)
Reagent (.RGT):	acetic acid ester
Note(s) (.COM):	Handbook
Reference(s):	

1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:

RX

Reaction ID (.ID): 5605719
Reactant BRN (.RBRN): 102415, 1696894, 380535
Reactant (.RCT): diazomethane, diethyl ether, 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester
Product (.PRO): 4.5.7-trimethoxy-phenoxazone-(2)-tetracarboxylic acid-(1.3.6.8)-methyl ester-(1)-triethyl ester-(3.6.8)
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 5605719.1
Reaction Classification (.CL): Chemical behaviour (half reaction)
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

Reaction:
RX
Reaction ID (.ID): 5484064
Reactant BRN (.RBRN): 506007, 380535
Reactant (.RCT): zinc dust, acetic acid, 1,7,9-trihydroxy-3-oxo-3H-phenoxazine-2,4,6,8-tetracarboxylic acid-2,6,8-triethyl ester
Product (.PRO): 2.4.5.7-tetraoxy-phenoxazine-tetracarboxylic acid-(1.3.6.8)-triethyl ester-(1.3.6)
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 5484064.1
Reaction Classification (.CL): Chemical behaviour (half reaction)
Note(s) (.COM): Handbook
Reference(s):
1. Leuchs, Justus Liebigs Ann. Chem., CODEN: JLACBF, 460, <1928>, 23

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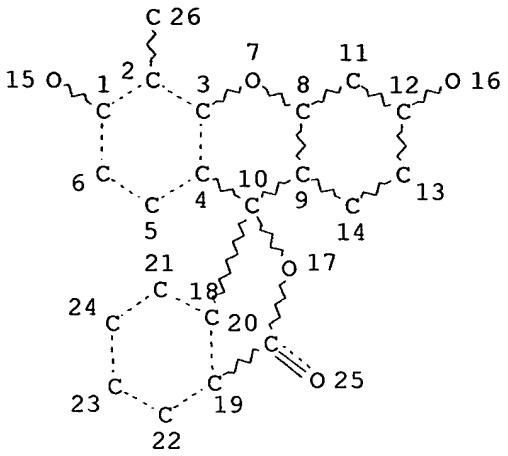
L58 STR



Considered
07/08/03
WSC

NODE ATTRIBUTES:
CONNECT IS E3 RC AT 2
CONNECT IS E3 RC AT 11
CONNECT IS M2 RC AT 26
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 18 19 20
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS UNLIMITED AT 18 19 20

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE
L60 49 SEA FILE=REGISTRY SSS FUL L58
L61 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L60

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L61 ANSWER 1 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:778611 HCAPLUS
DOCUMENT NUMBER: 137:275360
TITLE: Electrophoretic tag reagents comprising fluorescent compounds
INVENTOR(S): Matray, Tracy; Hernandez, Vincent; Singh, Sharat
PATENT ASSIGNEE(S): Aclara Biosciences, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 40 pp., Cont.-in-part of U.S. Ser. No. 698,846.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 2002146726	A1	20021010	US 2001-8495	20011109
US 6322980	B1	20011127	US 1999-303029	19990430
US 2001049105	A1	20011206	US 2001-824984	20010402
US 2001051340	A1	20011213	US 2001-824851	20010402
US 2002001808	A1	20020103	US 2001-825247	20010402
US 2002009737	A1	20020124	US 2001-824905	20010402
US 2002015954	A1	20020207	US 2001-825246	20010402
US 2002045738	A1	20020418	US 2001-825245	20010402
US 2002090616	A1	20020711	US 2001-825244	20010402

PRIORITY APPLN. INFO.: US 1999-303029 A2 19990430
US 2000-561579 B2 20000428
US 2000-602586 A2 20000621
US 2000-684386 A2 20001004
US 2000-698846 A2 20001027

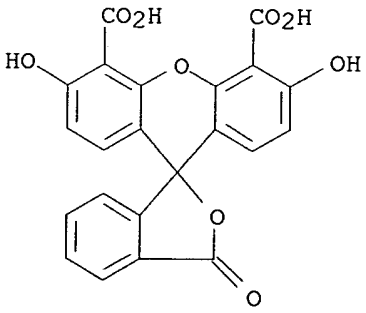
OTHER SOURCE(S): MARPAT 137:275360

AB The invention concerns electrophoretic probes comprising fluorescent compds. as detection groups and mobility modifiers which are disclosed for the multiplexed detection of the binding of, or interaction between, one or more ligands and target antiligands are provided. In one embodiment, detection involves the release of identifying tags as a consequence of target recognition. Target antiligands are contacted with a set of e-tag probes and the contacted antiligands are treated with a selected cleaving agent resulting in a mixt. of e-tag reporters. Typically, uncleaved or partially cleaved e-tag probes are removed and the mixt. of e-tag reporters is sepd. by any technique that provides for sepn. by mass or mass to charge ratio and the like and detected to provide for target identification.

IT **464914-28-1P**
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(electrophoretic tag reagents comprising fluorescent compds.)

RN 464914-28-1 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-ar,4',5'-tricarboxylic acid, 3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



D1—CO_2H

L61 ANSWER 2 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:755067 HCAPLUS
DOCUMENT NUMBER: 137:275359

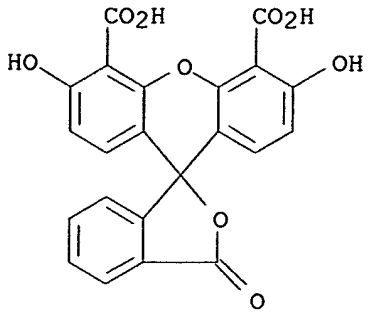
TITLE: Compositions and methods employing cleavable electrophoretic tag reagents
INVENTOR(S): Matray, Tracy; Hernandez, Vincent; Singh, Sharat
PATENT ASSIGNEE(S): Aclara Biosciences, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 42 pp., Cont.-in-part of U.S. Ser. No. 698,846.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002142329	A1	20021003	US 2001-8573	20011109
US 6322980	B1	20011127	US 1999-303029	19990430
US 2001049105	A1	20011206	US 2001-824984	20010402
US 2001051340	A1	20011213	US 2001-824851	20010402
US 2002001808	A1	20020103	US 2001-825247	20010402
US 2002009737	A1	20020124	US 2001-824905	20010402
US 2002015954	A1	20020207	US 2001-825246	20010402
US 2002045738	A1	20020418	US 2001-825245	20010402
US 2002090616	A1	20020711	US 2001-825244	20010402

PRIORITY APPLN. INFO.: US 1999-303029 A2 19990430
US 2000-561579 B2 20000428
US 2000-602586 A2 20000621
US 2000-684386 A2 20001004
US 2000-698846 A2 20001027
OTHER SOURCE(S): MARPAT 137:275359

AB The invention concerns probe sets for the multiplexed detection of the binding of, or interaction between, one or more ligands and target antiligands. Detection involves the release of identifying tags as a consequence of target recognition. The probe sets include electrophoretic tag probes or e-tag probes, comprising a detection region and a mobility-defining region called the mobility modifier, both linked to a target-binding moiety. Target antiligands are contacted with a set of e-tag probes and the contacted antiligands are treated with a selected cleaving agent resulting in a mixt. of e-tag reporters and uncleaved and/or partially cleaved e-tag probes. The mixt. is exposed to a capture agent effective to bind to uncleaved or partially cleaved e-tag probes, followed by electrophoretic sepn. In a multiplexed assay, different released e-tag reporters may be sepd. and detected providing for target identification. The methods employ compns. comprising luminescent mols. such as, for example, fluorescent mols., which are modified to provide for electrophoretic properties that differ for each modified luminescent mol. while maintaining substantially the same absorption, emission and quantum yield properties of the original luminescent mol. The compns. may be cleavably linked to binding mols. to form the e-tag probes.

IT **464914-28-1P**
RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(compns. and methods employing cleavable electrophoretic tag reagents)
RN 464914-28-1 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-ar,4',5'-tricarboxylic acid, 3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



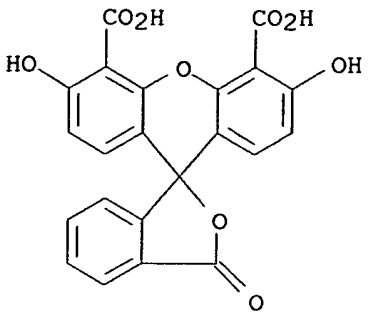
D1—CO_2H

L61 ANSWER 3 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:106271 HCAPLUS
DOCUMENT NUMBER: 136:295735
TITLE: Electrostatically Assembled Polyelectrolyte/Dendrimer Multilayer Films as Ultrathin Nanoreservoirs
AUTHOR(S): Khopade, Ajay J.; Caruso, Frank
CORPORATE SOURCE: Max Planck Institute of Colloids and Interfaces, Potsdam, D-14424, Germany
SOURCE: Nano Letters (2002), 2(4), 415-418
CODEN: NALEFD; ISSN: 1530-6984
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We report the prepn. of loadable ultrathin, multilayered polyelectrolyte/dendrimer films by the sequential electrostatic deposition of neg. charged poly(styrenesulfonate) (PSS) and a pos. charged fourth generation poly(amidoamine) dendrimer (4G PAMAM). Multilayers were first constructed on planar supports to examine their layer-by-layer growth. Quartz crystal microbalance (QCM) measurements showed regular growth for each layer deposited, while UV-Vis spectrophotometry revealed an adsorption-desorption trend to film formation, with partial PSS removal upon deposition of 4G PAMAM. PSS/4G PAMAM films were subsequently constructed on spherical latex colloids. Fluorescence spectroscopy showed that the films, when exposed to dye-contg. solns., acted as nano-reservoirs, sequestering the charged mols. from soln. due to the presence of the oppositely charged dendrimer. Release of the entrapped dye mols. was subsequently achieved by concn.-dependent diffusion in isotonic saline solns., illustrating the potential of the dendrimer-based films as systems for the uptake and release of various compds.

IT **407583-96-4**
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
(fluorescent probe; electrostatically assembled poly(styrenesulfonate) polyelectrolyte/PAMAM dendrimer multilayer films as potential controlled releases microcapsule)

RN 407583-96-4 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-dicarboxylic acid, 3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 4 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:51568 HCAPLUS
DOCUMENT NUMBER: 136:103838
TITLE: Fluorescein-based metal sensors and their use
INVENTOR(S): Lippard, Stephen J.; Burdette, Shawn; Hilderbrand, Scott; Tsien, Roger; Walkup, Grant
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002004562	A2	20020117	WO 2001-US41313	20010709
WO 2002004562	A3	20020530		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002106697	A1	20020808	US 2001-901466	20010709

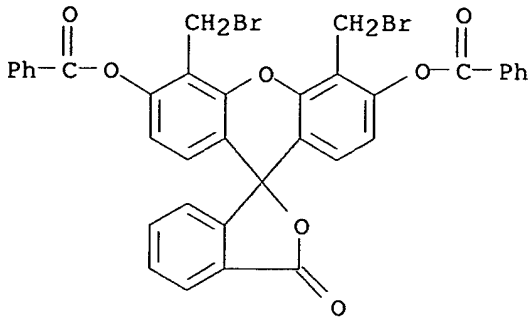
PRIORITY APPLN. INFO.:
US 2000-216872P P 20000707
US 2000-216875P P 20000707
US 2001-284384P P 20010417

OTHER SOURCE(S): MARPAT 136:103838

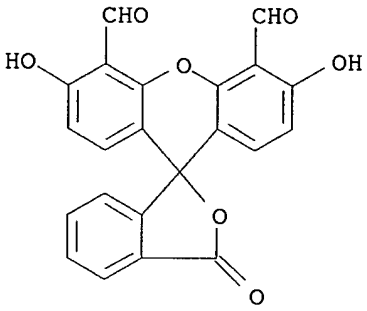
AB Fluorescein-based ligands are obtained for the detection of metal ions, such as zinc in intracellular media. In an example, an orange dye was produced by reductive amination of 4',5'-fluoresceindicarboxaldehyde with bis(2-pyridylmethyl)amine and shown to have a Zn-selective fluorescence response.

IT **357615-02-2P 357615-03-3P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prodn. of fluorescein-based metal sensors and their use)

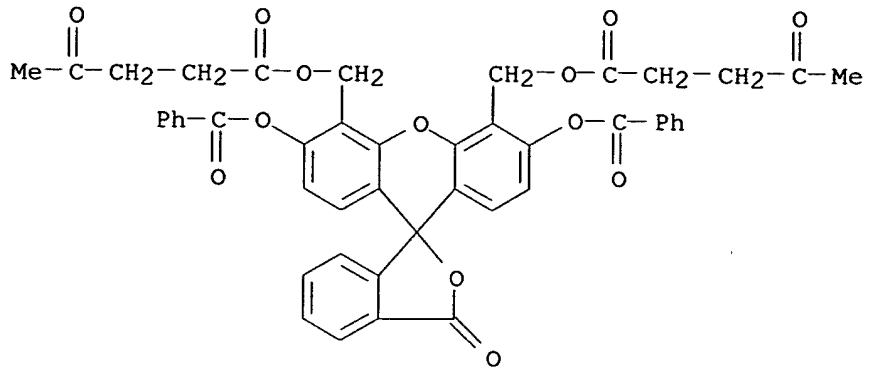
RN 357615-02-2 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(benzoyloxy)-4',5'-bis(bromomethyl)- (9CI) (CA INDEX NAME)



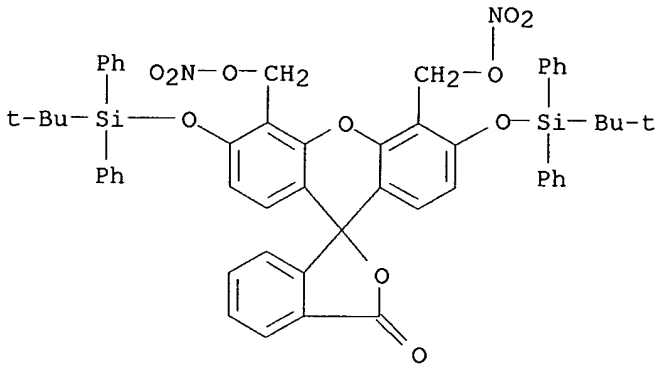
RN 357615-03-3 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-dicarboxaldehyde, 3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



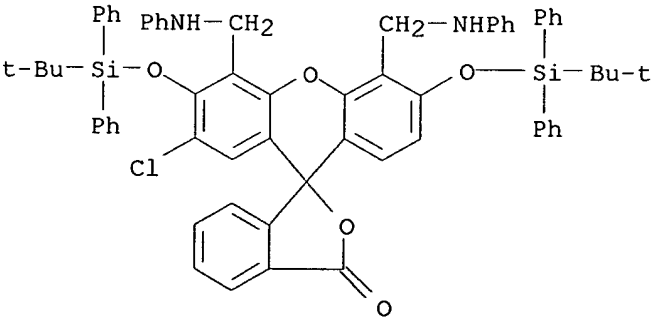
IT **389625-22-3P 389625-32-5P 389625-34-7P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prodn. of fluorescein-based metal sensors selective for zinc)
RN 389625-22-3 HCAPLUS
CN Pentanoic acid, 4-oxo-, [3',6'-bis(benzoyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl]bis(methylene) ester (9CI) (CA INDEX NAME)



RN 389625-32-5 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis[[(1,1-dimethylethyl)diphenylsilyl]oxy]-4',5'-bis[(nitrooxy)methyl]- (9CI) (CA INDEX NAME)



RN 389625-34-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 2'-chloro-3',6'-bis[[(1,1-dimethylethyl)diphenylsilyl]oxy]-4',5'-bis[(phenylamino)methyl]- (9CI) (CA INDEX NAME)

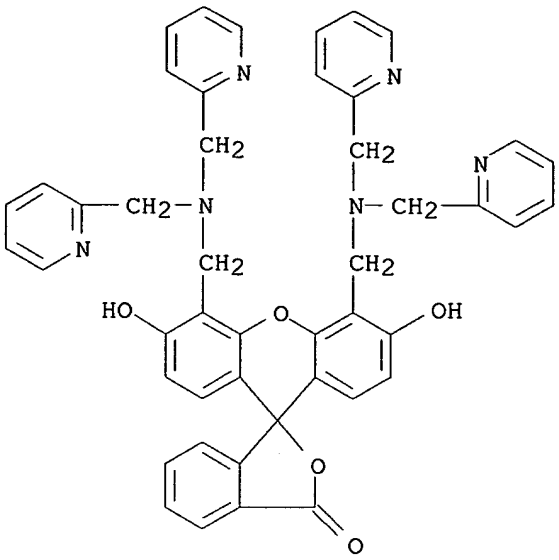


IT **357916-12-2P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material

use); PREP (Preparation); USES (Uses)
(orange dye; prodn. of fluorescein-based metal sensors and their use)

RN 357916-12-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)

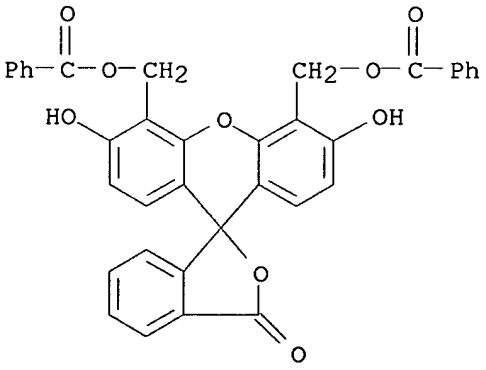


IT **389625-25-6P**

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(orange dye; prodn. of fluorescein-based metal sensors selective for zinc)

RN 389625-25-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[(benzoyloxy)methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



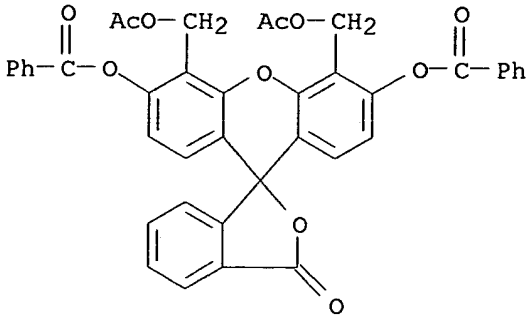
IT **389625-21-2P 389625-24-5P**

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(prodn. of fluorescein-based metal sensors selective for zinc)

RN 389625-21-2 HCAPLUS

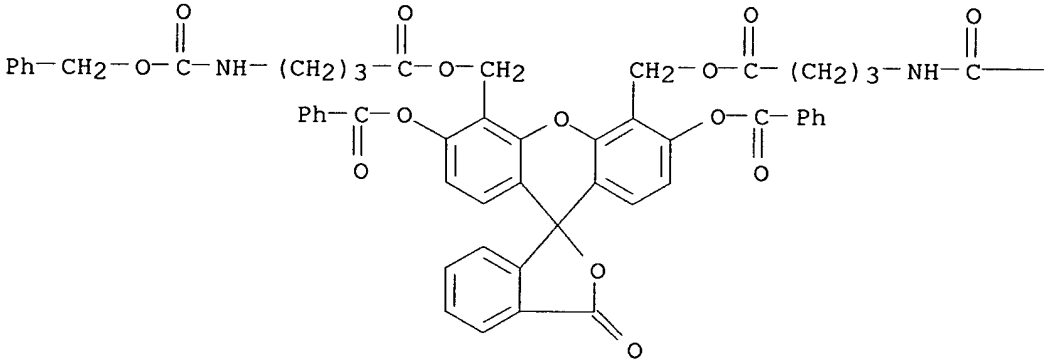
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[(acetyloxy)methyl]-3',6'-bis(benzoyloxy)- (9CI) (CA INDEX NAME)



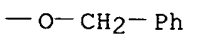
RN 389625-24-5 HCAPLUS

CN Butanoic acid, 4-[[(phenylmethoxy)carbonyl]amino]-, [3',6'-bis(benzoyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl]bis(methylene) ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT **288574-78-7P**

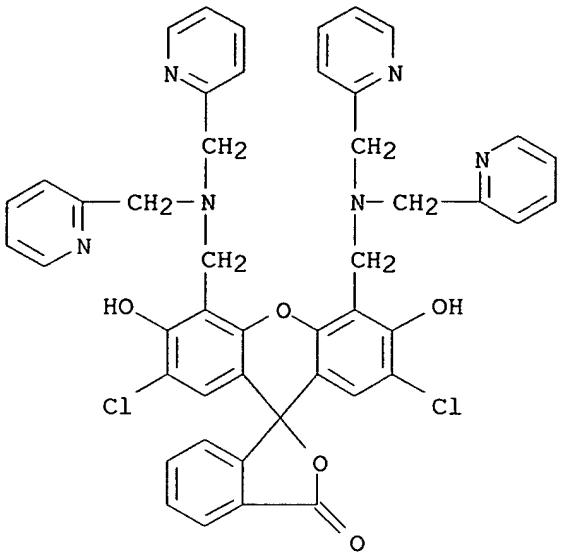
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(salmon pink dye; prodn. of fluorescein-based metal sensors selective for zinc)

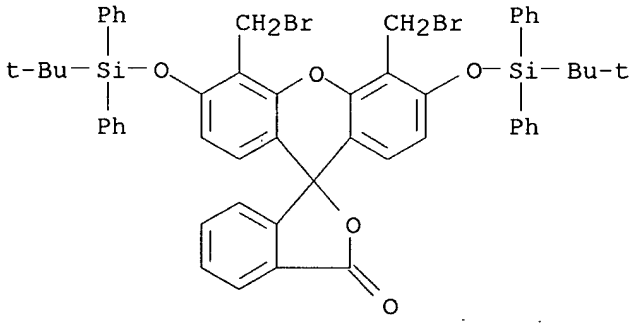
RN 288574-78-7 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA

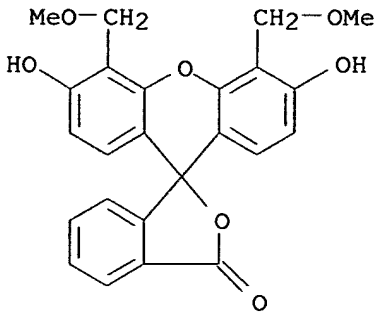
INDEX NAME)



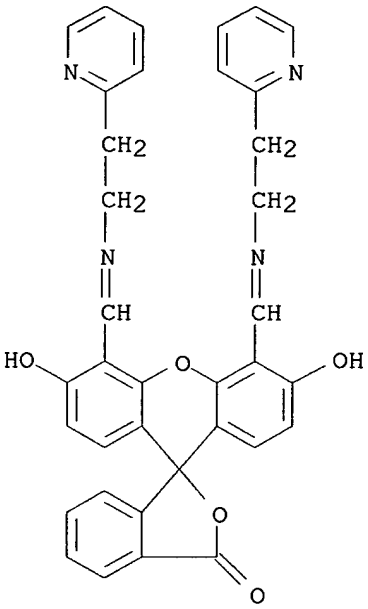
IT **389625-31-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prodn. of fluorescein-based metal sensors selective for zinc)
RN 389625-31-4 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis(bromomethyl)-3',6'-bis[[(1,1-dimethylethyl)diphenylsilyl]oxy]- (9CI) (CA INDEX NAME)



IT **389625-19-8P 389625-26-7P 389625-27-8P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(yellow dye; prodn. of fluorescein-based metal sensors selective for zinc)
RN 389625-19-8 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-4',5'-bis(methoxymethyl)- (9CI) (CA INDEX NAME)

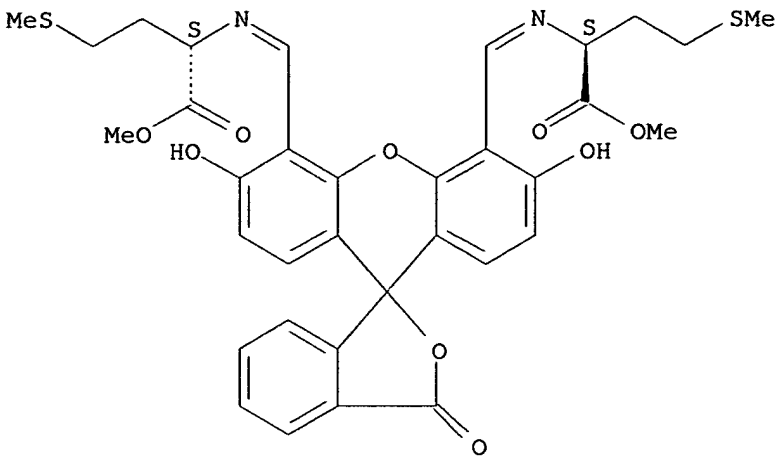


RN 389625-26-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-dihydroxy-4',5'-bis[[[2-(2-pyridinyl)ethyl]imino]methyl]- (9CI) (CA INDEX NAME)



RN 389625-27-8 HCAPLUS
CN L-Methionine, N,N'-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)dimethylidyne]bis-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



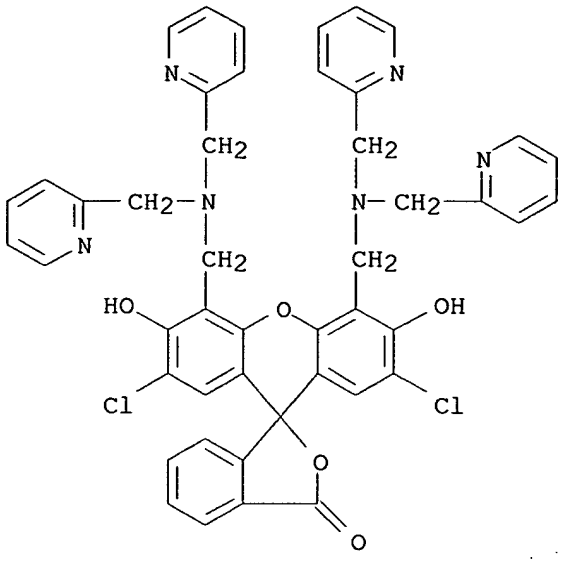
L61 ANSWER 5 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:530442 HCAPLUS
DOCUMENT NUMBER: 135:207684
TITLE: Fluorescent Sensors for Zn2+ Based on a Fluorescein Platform: Synthesis, Properties and Intracellular Distribution
AUTHOR(S): Burdette, Shawn C.; Walkup, Grant K.; Spingler, Bernhard; Tsien, Roger Y.; Lippard, Stephen J.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (2001), 123(32), 7831-7841
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two new fluorescent sensors for Zn2+ that utilize fluorescein as a reporting group, Zinpyr-1 and Zinpyr-2, have been synthesized and characterized. Zinpyr-1 is prepd. in one step via a Mannich reaction, and Zinpyr-2 is obtained in a multistep synthesis that utilizes 4',5'-fluorescein dicarboxaldehyde as a key intermediate. Both Zinpyr sensors have excitation and emission wavelengths in the visible range (.apprx.500 nm), dissocn. consts. (Kd1) for Zn2+ of <1 nM, quantum yields approaching unity (.PHI. = .apprx.0.9), and cell permeability, making them well-suited for intracellular applications. A 3- to 5-fold fluorescent enhancement is obsd. under simulated physiol. conditions corresponding to the binding of the Zn2+ cation to the sensor, which inhibits a photoinduced electron transfer (PET) quenching pathway. The x-ray crystal structure of a 2:1 Zn2+:Zinpyr-1 complex has also been solved, and is the first structurally characterized example of a complex of fluorescein substituted with metal binding ligands.

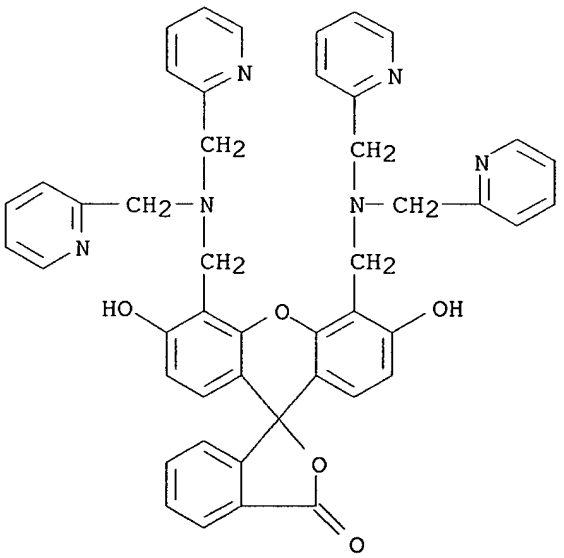
IT **288574-78-7P**, Zinpyr-1 **357916-12-2P**, Zinpyr 2
RL: NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(fluorescent sensors for Zn2+ based on fluorescein platform-synthesis, properties and intracellular distribution)

RN 288574-78-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-

pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)

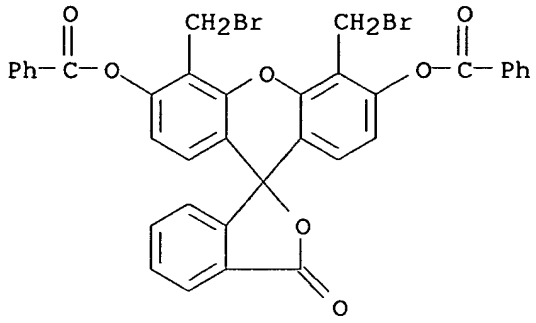


RN 357916-12-2 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)

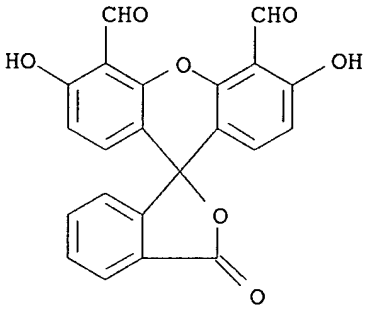


IT **357615-02-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxidn.)
RN 357615-02-2 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(benzoyloxy)-

4',5'-bis(bromomethyl)- (9CI) (CA INDEX NAME)



IT **357615-03-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with dipicolylamine)
RN 357615-03-3 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-dicarboxaldehyde, 3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



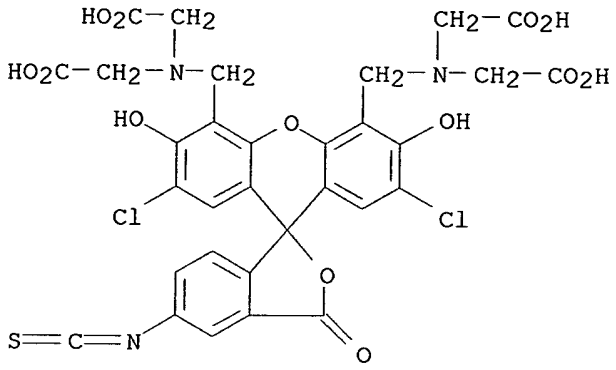
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 6 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:17002 HCAPLUS
DOCUMENT NUMBER: 134:219233
TITLE: A near-infrared luminescent label based on YbIII ions and its application in a fluoroimmunoassay
AUTHOR(S): Werts, Martinus H. V.; Woudenberg, Richard H.; Emmerink, Peter G.; van Gassel, Rob; Hofstraat, Johannes W.; Verhoeven, Jan W.
CORPORATE SOURCE: Laboratory of Organic Chemistry, University of Amsterdam, Amsterdam, 1018, Neth.
SOURCE: Angewandte Chemie, International Edition (2000), 39(24), 4542-4544
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This paper reports the interest in the use of rare earth lanthanide

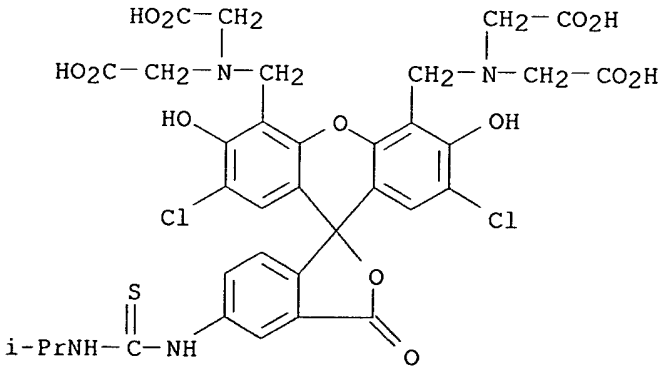
complexes as luminescent labels. 4',5'-Bis[N,N-bis(carboxymethyl)aminomethyl]-fluorescien (fluorexon, Fx) was found to be a very efficient sensitizer and a strongly binding ligand for near IR luminescent Yb(III) ion. The ligand FxITC which is structurally similar to Fx but carries an isothiocyanate group (ITC) that is reactive towards amino groups and so can be coupled to proteins. The iminodiacetic acid groups ensure firm complexation of lanthanide ions and the dicholorofluorescein chromophore acts as a sensitizer to near IR lanthanide luminescence. Thw label was tested in a simple heterogeneous noncompetitive immunoassay.

IT **212957-24-9P 329277-65-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(ytterbium based near IR luminescent label that can be conjugated with proteins and can be applied in model medical diagnostics)

RN 212957-24-9 HCAPLUS
CN Glycine, N,N'-[(2',7'-dichloro-3',6'-dihydroxy-5-isothiocyanato-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)



RN 329277-65-8 HCAPLUS
CN Glycine, N,N'-[[2',7'-dichloro-3',6'-dihydroxy-5-[[[(1-methylethyl)amino]thioxomethyl]amino]-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl]bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)



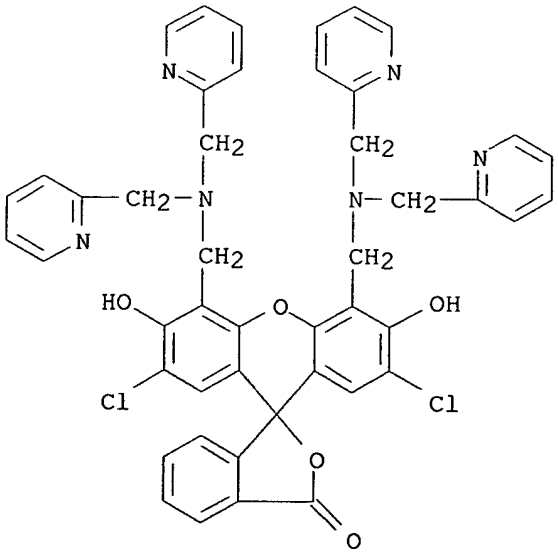
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

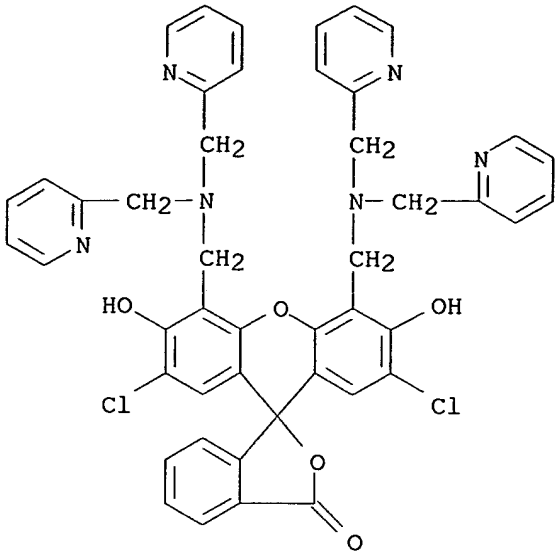
L61 ANSWER 7 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:356015 HCAPLUS
DOCUMENT NUMBER: 133:174121
TITLE: A New Cell-Permeable Fluorescent Probe for Zn2+
AUTHOR(S): Walkup, Grant K.; Burdette, Shawn C.; Lippard, Stephen J.; Tsien, Roger Y.
CORPORATE SOURCE: Department of Pharmacology and Chemistry and Biochemistry, Howard Hughes Medical Institute University of California at San Diego, La Jolla, CA, 92093-0647, USA
SOURCE: Journal of the American Chemical Society (2000), 122(23), 5644-5645
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors have prepd. a new, high affinity, selective fluorescent sensor, Zinpyr-1, for zinc that is membrane permeable. The fluorescein core of Zinpyr-1 exhibits bright fluorescence, can be excited at visible wavelengths, and overlaps well with the 488 nm Ar/ion laser line, which will facilitate confocal microscopy with this probe. Zinpyr-1 represents the first Zn2+ indicator to be developed in an ongoing program to tune the binding and optical properties of sensors for the neurosciences.

IT **288574-78-7P**, Zinpyr 1
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(Zinpyr 1; new cell-permeable fluorescent probe for Zn2+)

RN 288574-78-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[[bis(2-pyridinylmethyl)amino]methyl]-2',7'-dichloro-3',6'-dihydroxy- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

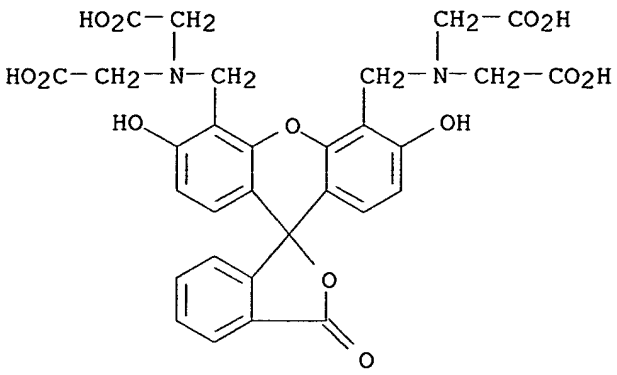
L61 ANSWER 8 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:100905 HCAPLUS
DOCUMENT NUMBER: 132:228111
TITLE: Spectrofluorimetric study of the complexes between calcein and lanthanide(III) ions
AUTHOR(S): Berregi, Inaki; Del Campo, Gloria; Durand, J. Senen; Casado, J. Alfonso
CORPORATE SOURCE: Unit of Analytical Chemistry, Faculty of Chemistry, University of the Basque Country, San Sebastian, 20080, Spain
SOURCE: Analytical Letters (2000), 33(2), 277-295
CODEN: ANALBP; ISSN: 0003-2719
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The equil. of calcein, an H6L type fluorescent ligand, with lanthanide(III) ions, Ln(III), was studied spectrofluorometrically in aq. soln. at const. ionic strength .mu.=0.1 (KCl), pH 8.0 and 25.0.+-.0.1.degree.. Application of the mole ratio and continuous variation methods reveals the formation of 1:1 complexes. The conditional stability consts. (.beta.') were calcd. from the anal. of the obsd. fluorescence vs. [Ln(III)]/[calcein] mole ratio data by using an iterative nonlinear least-squares computer program. The values obtained for .beta.' are in the range 5.24 .times. 106-5.77 .times. 107. The thermodn. stability consts. (.beta.) were estd. by calcg. the side-reaction coeffs. (.alpha.) for lanthanides and calcein. The .beta. values obtained were 3.2 .times. 1012-3.6 .times. 1013.

IT **207124-64-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(calcein; complex formation between calcein and lanthanide(III) ions by spectrofluorimetry)

RN 207124-64-9 HCAPLUS
CN Glycine, N,N'-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-

[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 9 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:618874 HCAPLUS
DOCUMENT NUMBER: 129:227809
TITLE: Diagnostic neodymium(III), ytterbium(III), or erbium(III) ion-ligand complexes
INVENTOR(S): Hofstraat, Johannes Willem
PATENT ASSIGNEE(S): Akzo Nobel N.V., Neth.
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9839654	A1	19980911	WO 1998-EP1287	19980228
WO 9839654	A3	20000106		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9868284	A1	19980922	AU 1998-68284	19980228
EP 968424	A1	20000105	EP 1998-913667	19980228
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE, FI				
US 20021875 63	A1	20021212	US 1999-380336	19991123

PRIORITY APPLN. INFO.: EP 1997-200615 A 19970303
US 1997-42354P P 19970324
WO 1998-EP1287 W 19980228

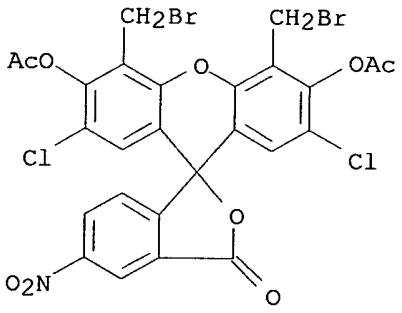
AB The invention relates to a method for detection of an analyte in a test sample by a specific binding reaction among the analyte, a specific

binding partner for the analyte, and an (immuno)reactant provided with a label, characterized in that the label is a lanthanide ion-ligand complex wherein the lanthanide ion is neodymium(III) ion (Nd3+), ytterbium(III) ion (Yb3+), or erbium(III) ion (Er3+) and the ligand comprises or is in contact with a sensitizing moiety which absorbs in the 400-1000 nm region, and preferably in the 400-800 nm region. Further, a diagnostic kit is disclosed as well as a method of detecting an analyte in a matrix of biomedical interest through an oligonucleotide, an antigen, or an antibody attached to a material, preferably core-shell latex or with specific binding sites wherein the antigen or antibody is labeled with the lanthanide ion-ligand complex and brought into contact with the analyte, after which the analyte with the lanthanide-ion complex is immobilized on the material, and, optionally, residual lanthanide-ion complex is removed, after which the sample obtained is irradiated with light in the 400-1000 nm region, and the emitted light from the sample is detected if the analyte is present in the matrix of biomedical interest. 2',7'-Dichloro-4',5'-fluorexon-4-isothiocyanate (prepn. given) was chelated with YbCl3.6H2O and used to label antibody to human chorionic gonadotropin for a sandwich immunoassay and amino-functionalized HIV oligonucleotide for a hybridization assay.

IT **212957-31-8P 212957-38-5P 212957-41-0P 212957-46-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diagnostic neodymium(III) and ytterbium(III) or erbium(III) ion-ligand complexes)

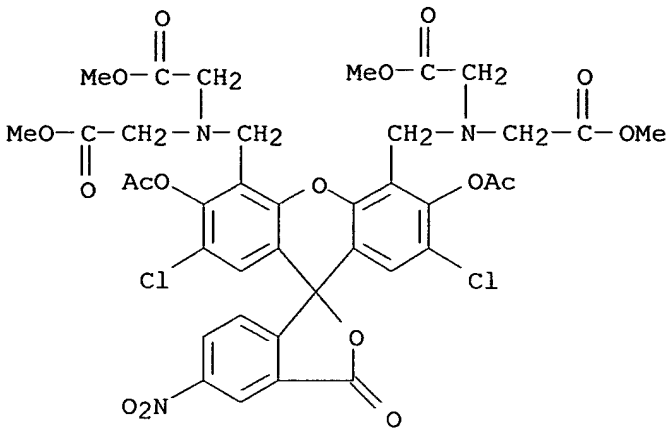
RN 212957-31-8 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(acetyloxy)-4',5'-bis(bromomethyl)-2',7'-dichloro-5-nitro- (9CI) (CA INDEX NAME)

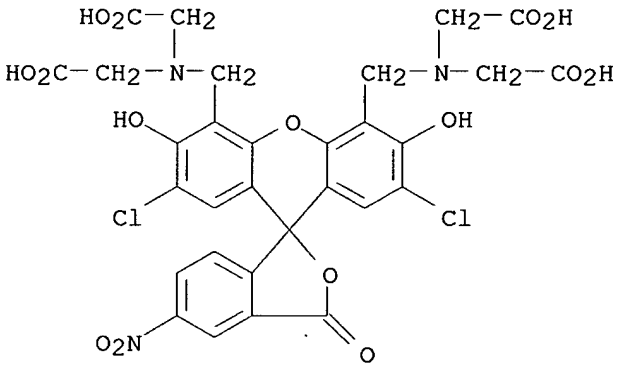


RN 212957-38-5 HCAPLUS

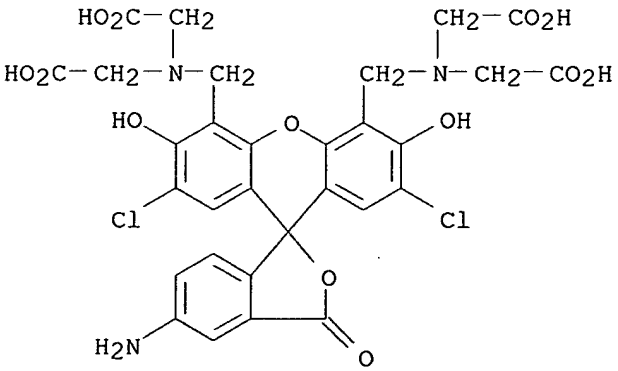
CN Glycine, N,N'-[[3',6'-bis(acetyloxy)-2',7'-dichloro-5-nitro-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl]bis(methylene)]bis[N-(2-methoxy-2-oxoethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

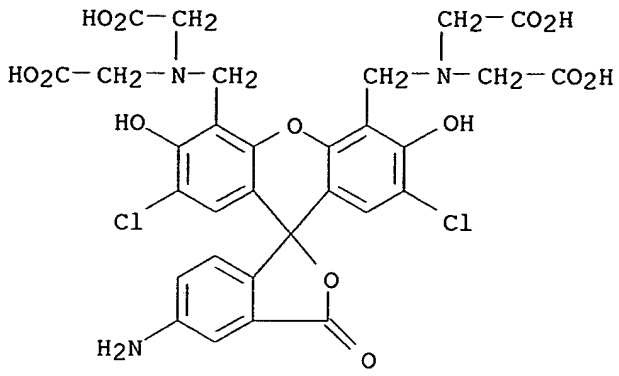


RN 212957-41-0 HCAPLUS
CN Glycine, N,N'-[(2',7'-dichloro-3',6'-dihydroxy-5-nitro-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)

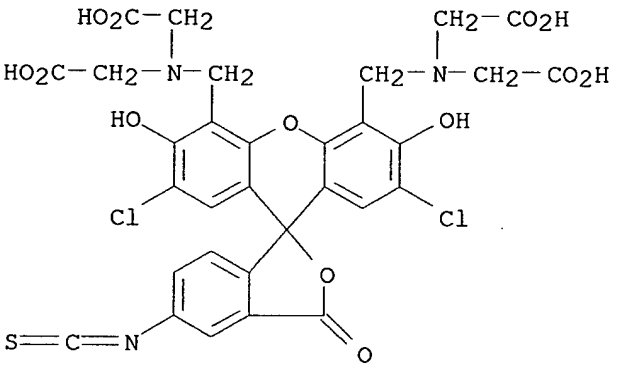


RN 212957-46-5 HCAPLUS
CN Glycine, N,N'-[(5-amino-2',7'-dichloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)





IT **212957-24-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and chelation of; diagnostic neodymium(III) and ytterbium(III) or erbium(III) ion-ligand complexes)
RN 212957-24-9 HCAPLUS
CN Glycine, N,N'-[(2',7'-dichloro-3',6'-dihydroxy-5-isothiocyanato-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)



L61 ANSWER 10 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:482695 HCAPLUS
DOCUMENT NUMBER: 121:82695
TITLE: Preparation of aromatic amines as petroleum cold flow additives
INVENTOR(S): Jackson, Graham; Kenward, Rachel Evelyn Mary; Brooke, Barbara Catherine
PATENT ASSIGNEE(S): Exxon Chemical Patents, Inc., USA
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9407842	A1	19940414	WO 1993-EP2739	19931005
W: AU, CA, FI, JP, KR, NO, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9351760	A1	19940426	AU 1993-51760	19931005
EP 663898	A1	19950726	EP 1993-922916	19931005
EP 663898	B1	19980624		
JP 08501783	T2	19960227	JP 1993-508733	19931005
AT 167664	E	19980715	AT 1993-922916	19931005
NO 9501309	A	19950529	NO 1995-1309	19950404
FI 9501588	A	19950602	FI 1995-1588	19950404
US 5667539	A	19970916	US 1996-698156	19960807

PRIORITY APPLN. INFO.: GB 1992-20876 A 19921005
WO 1993-EP2739 W 19931005
US 1995-392967 B1 19950517

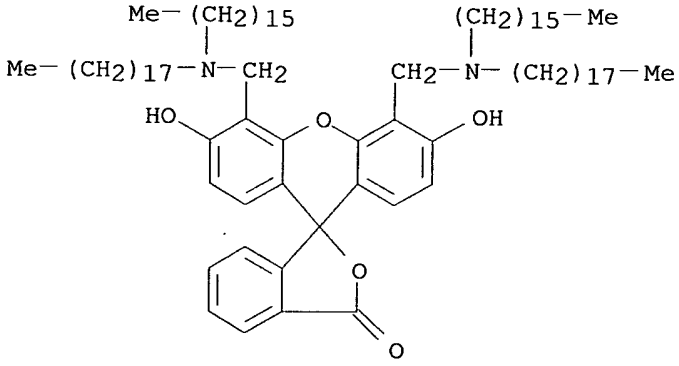
OTHER SOURCE(S): MARPAT 121:82695

AB B(ANR1R2)z [I; A = hydrocarbylene; B = substituted (polyvalent)arom. system; R1,R2 = C10-40 hydrocarbyl; 1 of R1,R2 may = H; Z = .gtoreq.1] were prepd. Data for compns. comprising I, e.g., II (R1,R2 = C16-22 hydrocarbyl) were given.

IT **156299-91-1P 156299-92-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as petroleum cold flow additive)

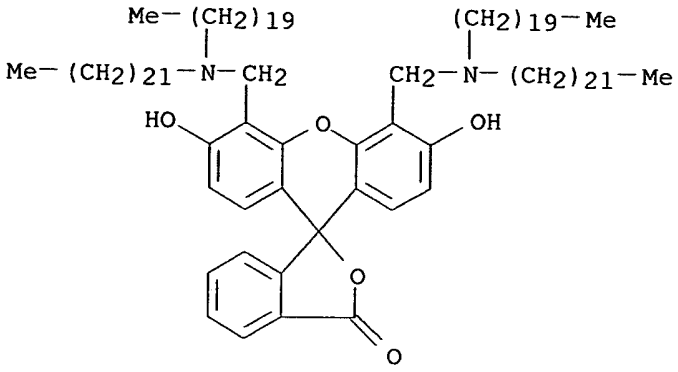
RN 156299-91-1 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[(hexadecyloctadecylamino)methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



RN 156299-92-2 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-bis[(docosyleicosylamino)methyl]-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



L61 ANSWER 11 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:51739 HCAPLUS
DOCUMENT NUMBER: 112:51739
TITLE: Fluorescein derivatives as stable fluorescent labels for liposomes
INVENTOR(S): Fiechtner, Michael D.; Bieniarz, Christopher; Shipchandler, Mohamed; Adamczyk, Maciej
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 297303	A2	19890104	EP 1988-108778	19880601
EP 297303	A3	19890920		
EP 297303	B1	19950315		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL				
US 4912208	A	19900327	US 1987-67833	19870629
AT 119904	E	19950415	AT 1988-108778	19880601
ES 2072253	T3	19950716	ES 1988-108778	19880601
CA 1295999	A1	19920218	CA 1988-570160	19880622
AU 8818482	A1	19890105	AU 1988-18482	19880628
AU 598385	B2	19900621		
JP 01022878	A2	19890125	JP 1988-162374	19880628
US 4970074	A	19901113	US 1989-367151	19890724

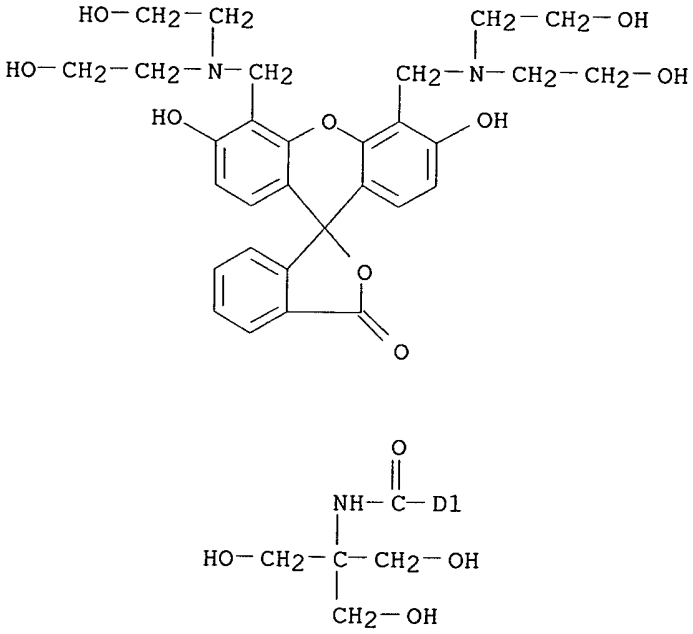
PRIORITY APPLN. INFO.: US 1987-67833 19870629
OTHER SOURCE(S): MARPAT 112:51739
AB Fluorescein derivs. I [R1 = pyridoxamide, COOH, XN(Y)(Z); R2, R3 = H, XN(Y)(Z); X = C:O, aminothiocarbonyl, methylene; Y = H, lower alkyl, carboxy alkyl, lower alkylol; Z = carboxy alkyl; lower alkylol, mono- or disaccharide, pyridoxyl] have a fluorescence spectrum and quantum yield characteristics similar to those of fluorescein. The compds. are readily synthesized and purified and are readily sol. in water at self-quenching concns. Due to the presence of polar polyhydroxy group substituents and the absence of metal-chelating groups, these fluorescein derivs. are susceptible to minimal leakage across liposome membranes and have fluorescence characteristics minimally sensitive to the presence of metal

ions. Compds. of the invention are thus exceptionally suitable for use in the development of highly storage stable liposome prepns. to be employed in immunolytic assays involving human body fluid samples. I (R1 = CON(CH3)CH2(CHOH)4CH2OH; R2 = R3 = H) (II; 5(6)-carboxyfluorescein-N-methylglucamide) was prepd. by reacting 5(6)-carboxyfluorescein-N-hydroxysuccinimide ester (prepd. from 5(6)carboxyfluorescein and N-hydroxysuccinimide) 95 with N-methyl-D-glucamine 39 and triethylamine 24 g in anhyd. HCON(CH3)2 for 12 h at room temp., followed by HPLC on silica gel using Me2CO:AcOH (50:1) with a 2-10% MeOH gradient. II in H2O (pH 7.2 with 6 N NaOH) and HEPES was added to a thin film of a mixt. of sphingomyelin:cholesterol:stearic acid (45:50:5) at 37.degree. for 15 min, vortexed, heated to 50.degree. and then slowly cooled to (2.degree./h) to 4.degree.. The liposomes were then washed and stored in isotonic buffer. Encapsulation of II after 121 days was 97.7%, compared to 95.9 and 41.2%, resp., for 5(6)-carboxyfluorescein and fluorescein.

IT **124452-57-9P 124452-58-0P 124452-59-1P**
124452-60-4P 124452-61-5P 124479-25-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as fluorescent labels for liposomes for immunoassays)

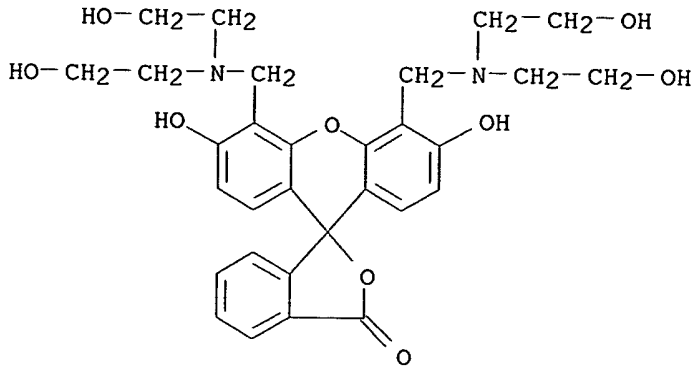
RN 124452-57-9 HCAPLUS

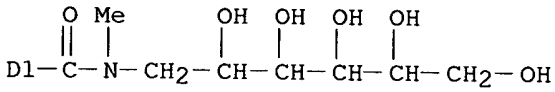
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]carboxamide, 4',5'-bis[[bis(2-hydroxyethyl)amino]methyl]-3',6'-dihydroxy-N-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-3-oxo- (9CI) (CA INDEX NAME)



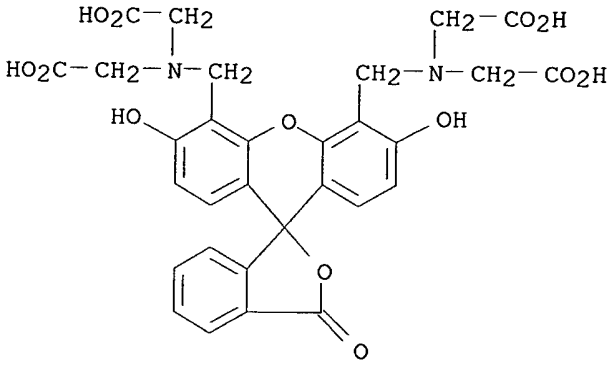
RN 124452-58-0 HCAPLUS

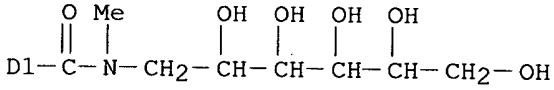
CN D-Glucitol, 1-[[[4',5'-bis[[bis(2-hydroxyethyl)amino]methyl]-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6(or 7)-yl]carbonyl]methylamino]-1-deoxy- (9CI) (CA INDEX NAME)



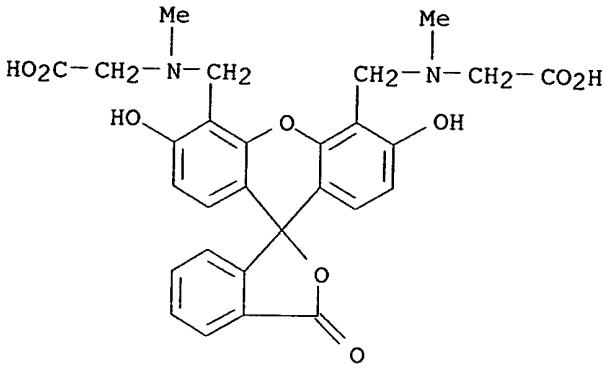


RN 124452-59-1 HCAPLUS
CN Glycine, N,N'-[[6(or 7)-[[(1-deoxy-D-glucitol-1-yl)methylamino]carbonyl]-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl]bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)



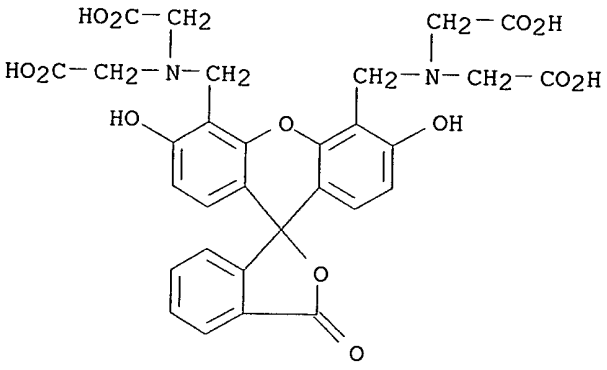


RN 124452-60-4 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]carboxylic acid, 4',5'-bis[[(carboxymethyl)methylamino]methyl]-3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)



D1—CO_2H

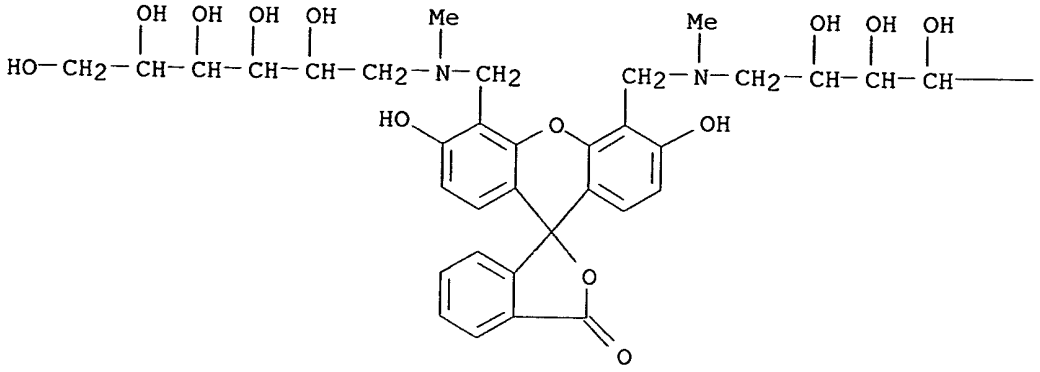
RN 124452-61-5 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]carboxylic acid, 4',5'-bis[[bis(carboxymethyl)amino]methyl]-3',6'-dihydroxy-3-oxo- (9CI) (CA INDEX NAME)

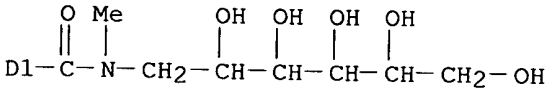


D1—CO_2H

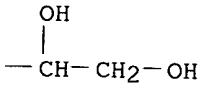
RN 124479-25-0 HCAPLUS
CN D-Glucitol, 1,1'-[[6(or 7)-[[(1-deoxy-D-glucitol-1-yl)methylamino]carbonyl]-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl]bis[methylene(methylimino)]]bis[1-deoxy- (9CI) (CA INDEX NAME)

PAGE 1-A





PAGE 1-B



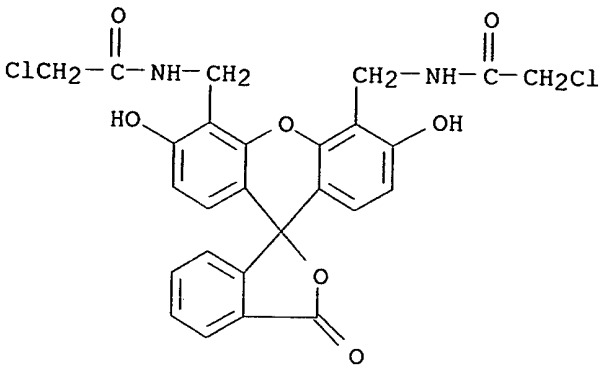
L61 ANSWER 12 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:33213 HCAPLUS
DOCUMENT NUMBER: 106:33213
TITLE: A revised structure of fluorescein mercuric acetate
AUTHOR(S): Shipchandler, M. T.; Fino, J. R.
CORPORATE SOURCE: Diagnost. Div., Abbott Lab., Abbott Park, IL, 60064, USA
SOURCE: Analytical Biochemistry (1986), 154(2), 576-7
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English

AB With the help of NMR spectroscopy the structure assignment of fluorescein mercuric acetate, previously assigned as 2',7'-bis(acetoxymercury)fluorescein, is cor. to 4',5'-bis(acetoxymercury)fluorescein.

IT **106178-25-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR of)

RN 106178-25-0 HCAPLUS

CN Acetamide, N,N'-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[2-chloro- (9CI) (CA INDEX NAME)



L61 ANSWER 13 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:128372 HCAPLUS
DOCUMENT NUMBER: 102:128372
TITLE: Fluorescent polymeric microspheres and method of linking them to biologically active proteins
PATENT ASSIGNEE(S): Yeda Research and Development Co. Ltd., Israel
SOURCE: Israeli, 12 pp.
CODEN: ISXXAQ
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IL 61910	A1	19840831	IL 1981-61910	19810115

PRIORITY APPLN. INFO.: IL 1981-61910 19810115

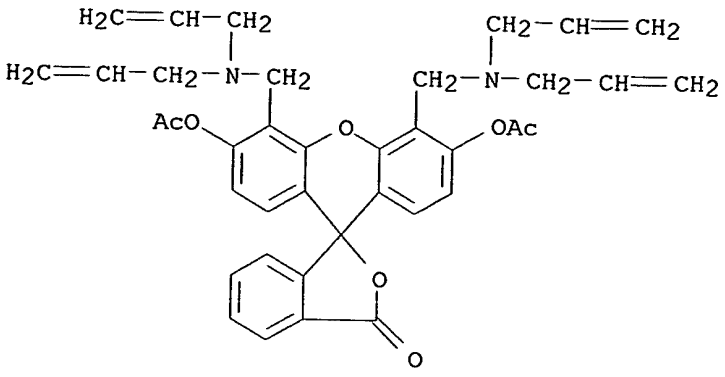
AB Methods are described for prepg. fluorescent microspheres and coupling them to biol. active proteins (e.g., antibodies, antigens, or hormones). These microspheres comprise an acrylate or acrylamide type polymer produced from 1 or 2 monomers (e.g., methylmethacrylate, N,N'-methylene bis-acrylamide). Microspheres were then activated with diamine (e.g., ethylene diamine) and reacted with glutaraldehyde for providing linking groups for proteins or other ligands. For example, fluorescent microspheres were prepd., coupled with Ig, and attached to cell; cells were then detected and sorted by fluorescence-based methods.

IT **95522-47-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(microspheres, prepn. and linking to biol. active proteins)

RN 95522-47-7 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 3',6'-bis(acetyloxy)-4',5'-bis[(di-2-propenylamino)methyl]spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one and N,N'-methylenebis[2-propenamide] (9CI) (CA INDEX NAME)

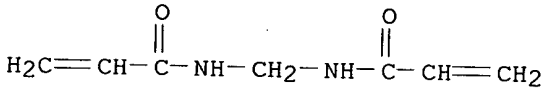
CM 1

CRN 85713-99-1
CMF C38 H38 N2 O7



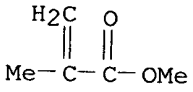
CM 2

CRN 110-26-9
CMF C7 H10 N2 O2

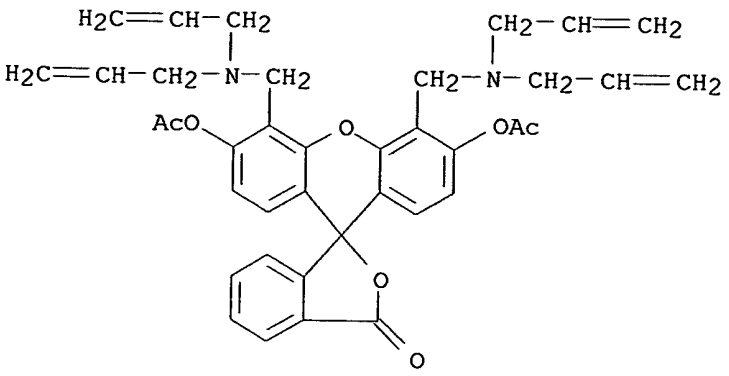


CM 3

CRN 80-62-6
CMF C5 H8 O2



IT **85713-99-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for fluorescent polymeric microspheres prepn.)
RN 85713-99-1 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(acetyloxy)-4',5'-bis[(di-2-propenylamino)methyl]- (9CI) (CA INDEX NAME)

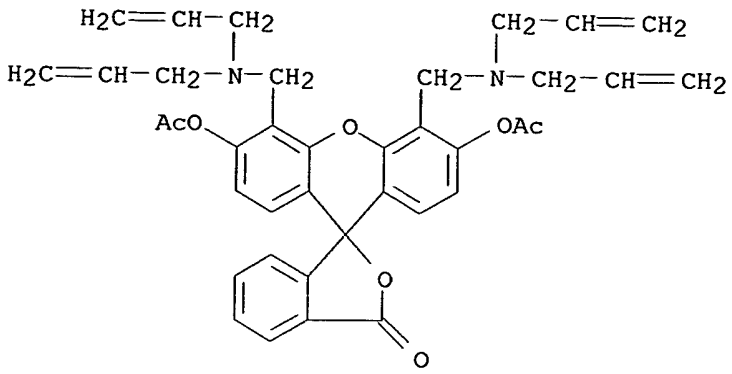


L61 ANSWER 14 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:194334 HCAPLUS
DOCUMENT NUMBER: 98:194334
TITLE: The selective detection of cell surface determinants by means of antibodies and acetylated avidin attached to highly fluorescent polymer microspheres
AUTHOR(S): Kaplan, Miriam R.; Calef, Edna; Bercovici, Tuvia; Gitler, Carlos
CORPORATE SOURCE: Dep. Membr. Res., Weizmann Inst. Sci., Rehovot, Israel
SOURCE: Biochimica et Biophysica Acta (1983), 728(1), 112-20
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Procedures are described for the synthesis of 500-.ANG.-diam. polymer microspheres contg. a novel fluorescent crosslinking agent. These microspheres have very high fluorophore concn. without quenching of the fluorescence and show very low nonspecific interaction with cells. When monoclonal anti-Thy-1.2 is attached to the fluorescent microspheres, specific binding results in 104 spheres being attached per thymocyte while nonspecific binding is <1%. Similar values are obtained for an indirect staining procedure. The high nonspecific binding of cationic avidin to neg. cell surfaces is decreased to negligible levels by acetylation of the amine groups of the protein without decreasing its high-affinity binding to biotin. The use of acetyl-avidin (pI = 6.7) directly, or when attached to fluorescent microspheres, resulted in a highly selective detection of biotinyl groups on the erythrocyte or lymphocyte cell surface. Attachment of biotinyl groups to the hinge carbohydrates of antibodies did not affect their specificity. It allowed their detection by means of microspheres-acetyl-avidin conjugates.

IT **85713-99-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with methylmethacrylate and with ethylenediamine or hydrazine hydrate)

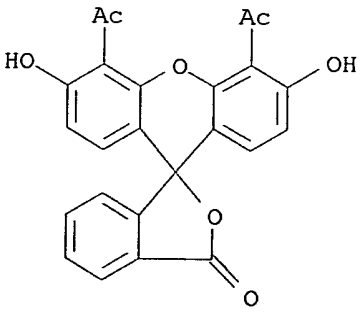
RN 85713-99-1 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 3',6'-bis(acetyloxy)-4',5'-bis[(di-2-propenylamino)methyl]- (9CI) (CA INDEX NAME)



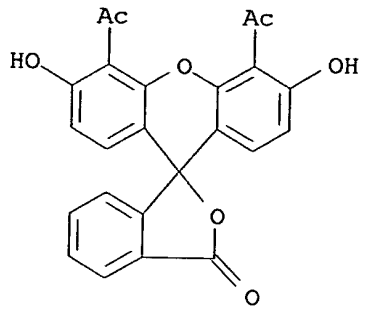
L61 ANSWER 15 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1972:126711 HCAPLUS
DOCUMENT NUMBER: 76:126711
TITLE: Friedel-Crafts reaction. XI. .gamma.-Substitution in the synthesis of fluoresceins
AUTHOR(S): Desai, R. D.; Desai, B. M.; Chandrasekhar, T. R.; Maraballi, M. S.
CORPORATE SOURCE: Mafatlal Gagalbhai Sci. Inst., Ahmedabad, India
SOURCE: Journal of the Indian Chemical Society (1971), 48(12), 1079-82
CODEN: JICSAH; ISSN: 0019-4522
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2,6-(HO)2C6H3Ac was treated with phthalic anhydride and AlCl3 to give the fluorescein (I). 3-Nitrophthalic anhydride was treated with m-(HO)2C6H4 and H2SO4 or with 2,6-(HO)2C6H3Ac and AlCl3 to give analogs of I. 2,4-(HO)2C6H3-CO2H was treated with AlCl3 and phthalic anhydride to give II. Analogs of II were prepd. by treating phthalic anhydride or 3-nitrophthalic anhydride with AlCl3 and 2,4-(HO)2C6H3CO2H, 2,4-(HO)2C6H3CO2Me, 2,4-(HO)2C6H3CONH2, or 2,4(HO)2C6H3Ac.

IT **35784-47-5P 36349-52-7P 36423-65-1P 36423-66-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35784-47-5 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-diacetyl-3',6'-dihydroxy- (9CI) (CA INDEX NAME)

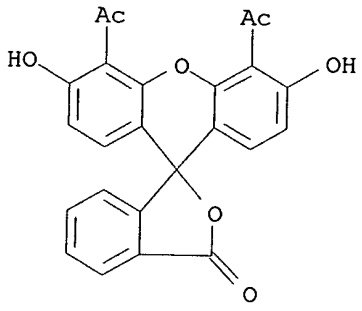


RN 36349-52-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-diacetyldibromo-3',6'-dihydroxy- (9CI) (CA INDEX NAME)



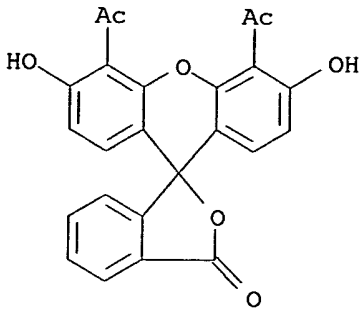
2 (D1—Br)

RN 36423-65-1 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-diacetyl-3',6'-dihydroxy-4(or 7)-nitro- (9CI) (CA INDEX NAME)



D1—NO_2

RN 36423-66-2 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one, 4',5'-diacetyldibromo-3',6'-dihydroxy-4(or 7)-nitro- (9CI) (CA INDEX NAME)



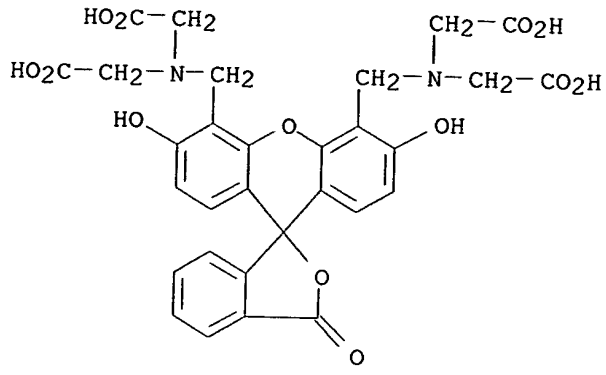
D1—NO_2

2 (D1—Br)

L61 ANSWER 16 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1972:107534 HCAPLUS
DOCUMENT NUMBER: 76:107534
TITLE: Statocalcein, a stable Calcein indicator for the EDTA titration of calcium
AUTHOR(S): Hoyle, William C.; Diehl, Harvey
CORPORATE SOURCE: Dep. Chem., Iowa State Univ., Ames, IA, USA
SOURCE: Talanta (1972), 19(2), 206-7
CODEN: TLNTA2; ISSN: 0039-9140
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Statocalcein, i.e. K2Ca5L2 (H6L = Calcein) was more stable in Calcein and was recommended as indicator for the fluorimetric titrn. of Ca with EDTA. Statocalcein solns. were stable .gtoreq.210 days and gave sharp end points for titrns. carried out in a darkened room. When using 40.02 ml of 0.0125M EDTA for a titrn., the std. deviation was 0.03-0.04 ml.

IT **36352-49-5**
RL: ANST (Analytical study)
(indicator for EDTA titrn. of calcium)
RN 36352-49-5 HCAPLUS
CN Glycine, N,N'-[(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4',5'-diyl)bis(methylene)]bis[N-(carboxymethyl)-, calcium potassium salt (2:5:2) (9CI) (CA INDEX NAME)



● 5/2 Ca

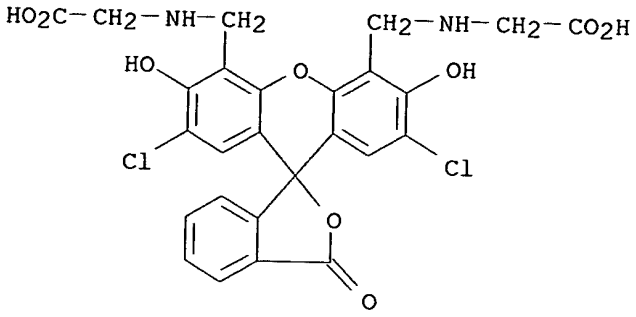
● K

L61 ANSWER 17 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:139230 HCAPLUS
DOCUMENT NUMBER: 72:139230
TITLE: Analytical applications of chelating agents. LII. Fluorescence of some fluorescein dyes and their application as metal-fluorescent indicators
AUTHOR(S): Bermejo-Martinez, Francisco; Gonzalez de Lopidana, Monserrat G.
CORPORATE SOURCE: Fac. Cienc., Univ. Santiago de Compostela, Santiago de Compostela, Spain
SOURCE: Informacion de Quimica Analitica (1969), 23(6), 151-5, 188
CODEN: IFQAAZ; ISSN: 0367-777X
DOCUMENT TYPE: Journal
LANGUAGE: Spanish

AB Fluorescence was measured of bis-N,N-glycinemethylene-3,6-dichloro fluorescein [25639-38-7] (I), bis-2',7'-N,N-glycinemethylene-4',5'-dichlorofluorescein [21666-05-7], bis-N,N-glycinemethylenefluorescein [25639-40-1], bis-4',5'-N,N-glycinemethylene-2',7'-dichlorofluorescein [**21667-31-2**], and bis-N-N,-glycinemethylene-4,5-dichlorofluorescein [25639-39-8] in aq. soln. On excitation at 366 m.mu., all exhibited emission with a max. at 525 m.mu.. Position of the max. was independent of pH. Relative intensities were 100, 71, 35, 32, and 10, resp., at pH 5.7. Max. fluorescence of I was obsd. at pH 4.8. In acid soln., fluorescence of I was independent of excitation wavelength 366 or 480 .mu.m. In alk. soln., fluorescence intensity of I was greater with 480 m.mu. excitation than with 366 m.mu. excitation. Fluorescence of the other dyes behaved similarly. The decrease in fluorescence intensity with increasing concn. of Cu2+ indicates I forms a 1:1 complex with Cu2+.

IT **21667-31-2**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (as metal-fluorescent indicators)

RN 21667-31-2 HCAPLUS
CN Fluorescein, 4',5'-bis[[(carboxymethyl)amino]methyl]-2',7'-dichloro- (8CI) (CA INDEX NAME)

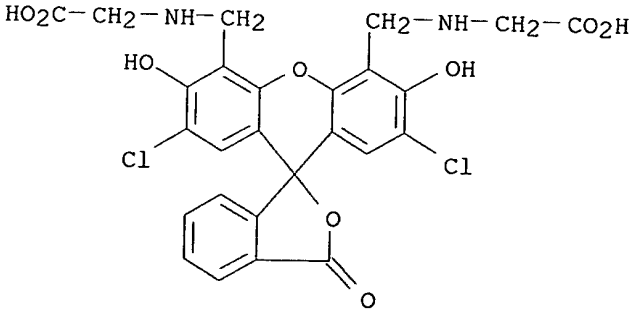


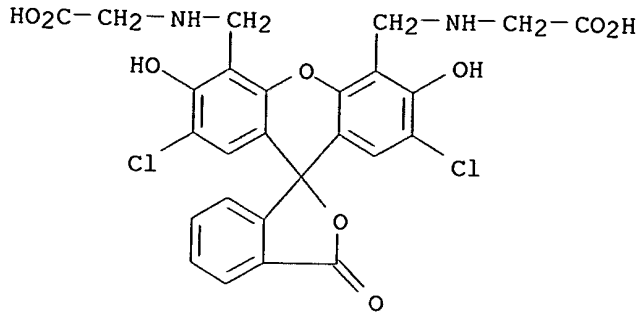
L61 ANSWER 18 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1969:456243 HCAPLUS
DOCUMENT NUMBER: 71:56243
TITLE: Analytical applications of chelons. XLIX. Metallofluorescent indicators
AUTHOR(S): Bermejo Martinez, Francisco; Gonzalez de Lopidana, Monserrat G.
CORPORATE SOURCE: Univ. Santiago/Compostela, Santiago/Compostela, Spain
SOURCE: Analytica Chimica Acta (1969), 47(1), 139-44
CODEN: ACACAM; ISSN: 0003-2670
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Four new metallofluorescent indicators, analogous to calcein but prepd. from glycine instead of iminodiacetic acid, have been synthesized and studied by thin-layer chromatog. In addn. to fluorescein itself, 3 isomers of dichlorofluorescein were used in the syntheses. The product obtained with 2',7'-dichlorofluorescein, 4',5'-bis(carboxymethylamino-methyl)-2',7'-dichlorofluorescein, is recommended as a fluorescent indicator for the titrn. of Cu(II) with EDTA solns.

IT **21667-31-2**
RL: ANST (Analytical study)
(as chelatometric indicator)

RN 21667-31-2 HCAPLUS
CN Fluorescein, 4',5'-bis[[(carboxymethyl)amino]methyl]-2',7'-dichloro- (8CI) (CA INDEX NAME)



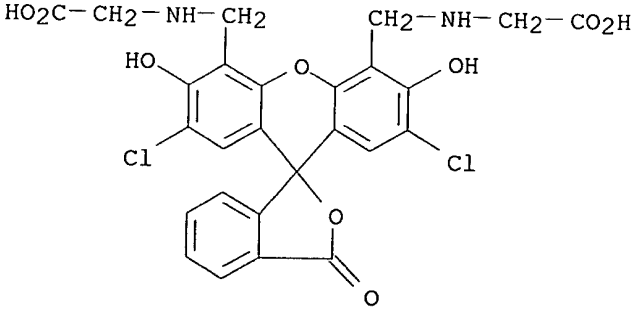


L61 ANSWER 19 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1968:408009 HCAPLUS
DOCUMENT NUMBER: 69:8009
TITLE: Metallofluorescent indicators
AUTHOR(S): De Lopidana, Montserrat Gras G.
CORPORATE SOURCE: Univ. Santiago, Santiago, Spain
SOURCE: Acta Cientifica Compostelana (1966), 3(4), 173-80
CODEN: ACCCAW; ISSN: 0567-7378
DOCUMENT TYPE: Journal
LANGUAGE: Spanish

AB 2',7'-Bis[[bis(carboxymethyl)amino]methyl]-4', 5'-dichlorofluorescein, 4',5'-bis[[bis(carboxymethyl)amino]methyl]-2',7' -dichlorofluorescein and a bis[[bis(carboxymethyl)amino]methyl] - 3,6 - dichlorofluorescein (I) were prepd. The products were sepd. chromatographically from the rest of the initial components and accompanying products. The absorptivity of the fluorescence of the 3 indicators on addn. of Cu was studied in uv light at pH 3.7-10. The fluorescence is most intense at pH 5.5-6.5; the use of pH 5.5 is recommended. A 2nd, smaller max. of fluorescence occurs for I at pH 9.3. Contents of Cu detd. with use of these indicators agree with values detd. with use of EDTA within the limits of .+-.0.2-0.4%. The max. of emission of the indicators lies at 525 m.mu., for excitation at 366 m.mu.. Cu forms a 1:1 complex with I.

IT **21667-31-2**
RL: ANST (Analytical study)
(in detn. of copper)

RN 21667-31-2 HCAPLUS
CN Fluorescein, 4',5'-bis[[(carboxymethyl)amino]methyl]-2',7'-dichloro- (8CI) (CA INDEX NAME)

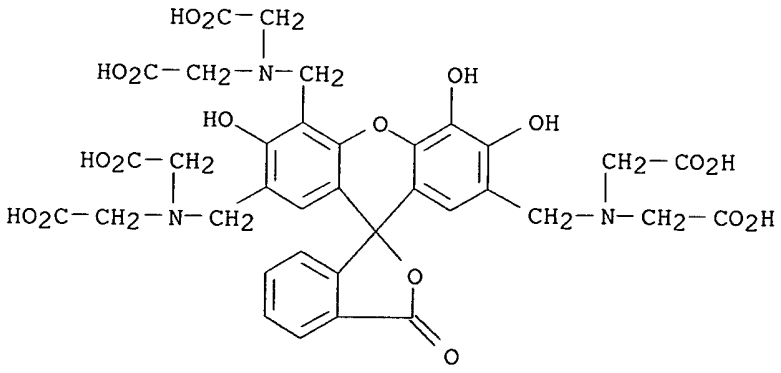


L61 ANSWER 20 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1965:471847 HCAPLUS
DOCUMENT NUMBER: 63:71847
ORIGINAL REFERENCE NO.: 63:13210f-h
TITLE: Hydroxyfluoran and its derivatives as organic reagents. II. Syntheses of chlorohydroxyfluoran derivatives and hydroxyfluoran complexones
AUTHOR(S): Mori, Itsuo
CORPORATE SOURCE: Coll. Pharm., Gifu, Japan
SOURCE: Yakugaku Zasshi (1965), 85(6), 561-4
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

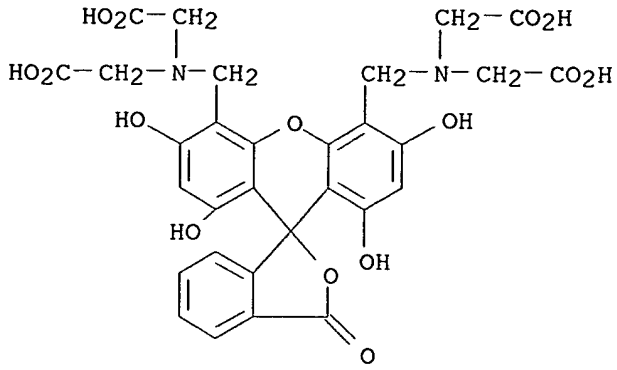
AB cf. CA 63, 6954d. o-(5-Chloro-2,4-dihydroxybenzoyl)benzoic acid (1.0 g.), 0.55 g. 1-naphthol, and 1 g. ZnCl2 was heated at 170-80.degree. 1 hr., dissolved in 5% NaOH, filtered, and the filtrate neutralized with 30% AcOH and washed with H2O to give 75.4% 5',7'-dichloro-6'-hydroxy-3',4'-benzofluoran, red, m. 278-91.degree.. Similarly prepd. were 5',7'-dichloro-6'-hydroxy-2',3'-benzofluoran (dark brown, m. 270-85.degree.), 6'-hydroxy-7'-chloro-2',3'-benzofluoran (dark brown, m. 288-99.degree.), 6'-hydroxy-7'-chloro-3',4'-benzofluoran (dark red, m. 284-95.degree.), 4',5'-dichloro-2',3',6',7'-tetrahydroxyfluoran (orange brown, m. 285-300.degree.), 2',7'-dichloro-3',4',5',6'-tetrahydroxyfluoran (dark brown, m. 280-96.degree.), and 4',5'-dichloro-1',3',6',8'-tetrahydroxyfluoran (light brown, m. 229-35.degree.). Also were prepd. hydroxyfluoran compds. with iminoacetic acid and iminodiacetic acid.

IT **5070-22-4**, Fluoran, 2',4',7'-tris[[bis(carboxymethyl)amino]-methyl]-3',5',6'-trihydroxy- **5119-27-7**, Fluoran, 4',5'-bis[[bis(carboxymethyl)amino]methyl]-1',3',6',8'-tetrahydroxy- **5143-11-3**, Fluoran, 4',5'-bis[[(carboxymethyl)amino]methyl]-2',3',6',7'-tetrahydroxy- **5188-44-3**, Fluoran, 2',4',5',7'-tetrakis[[bis(carboxymethyl)-amino]methyl]-1',3',6'-trihydroxy- **5489-73-6**, Fluoran, 4',5'-bis[[bis(carboxymethyl)amino]methyl]-2',3',6',7'-tetrahydroxy- **6023-01-4**, Fluoran, 4',5'-bis[[(carboxymethyl)amino]methyl]-1',3',6',8'-tetrahydroxy- **105840-96-8**, Fluoran, 2',4',5'-tris[[bis(carboxymethyl)amino]-methyl]-1',3',6'-trihydroxy-(?)
(prepn. of)

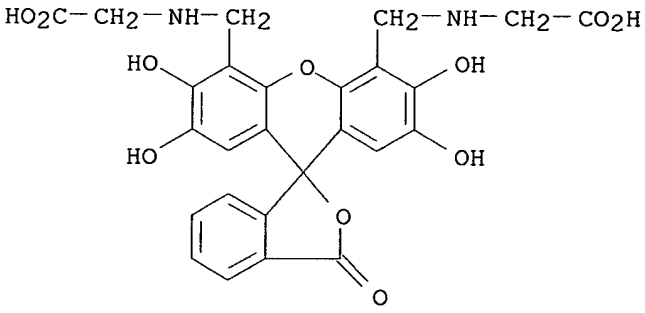
RN 5070-22-4 HCAPLUS
CN Acetic acid, [(3',5',6'-trihydroxy-3-oxospiro[phthalan-1,9'-xanthene]-2',4',7'-triyl)tris(methylenenitrilo)]hexa- (8CI) (CA INDEX NAME)



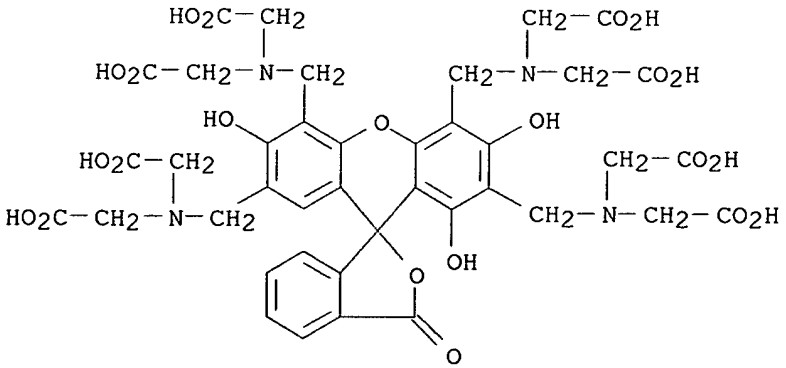
RN 5119-27-7 HCAPLUS
CN Acetic acid, [(1',3',6',8'-tetrahydroxyspiro[phthalan-1,9'-xanthene]-4',5'-diyl)bis(methylenenitrilo)]tetra- (8CI) (CA INDEX NAME)

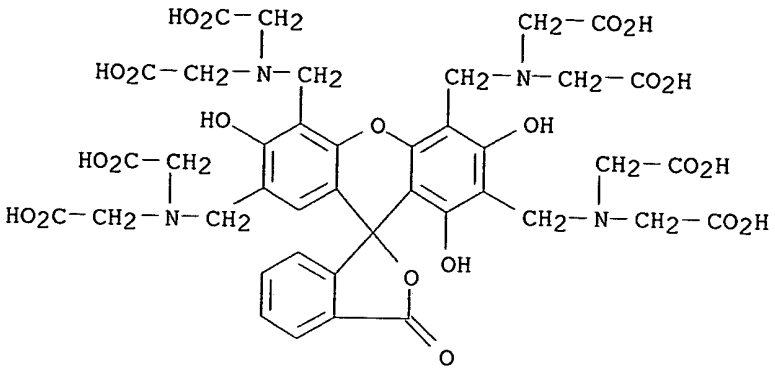


RN 5143-11-3 HCAPLUS
CN Glycine, N,N'-[(2',3',6',7'-tetrahydroxyspiro[phthalan-1,9'-xanthene]-4',5'-diyl)dimethylene]di- (8CI) (CA INDEX NAME)

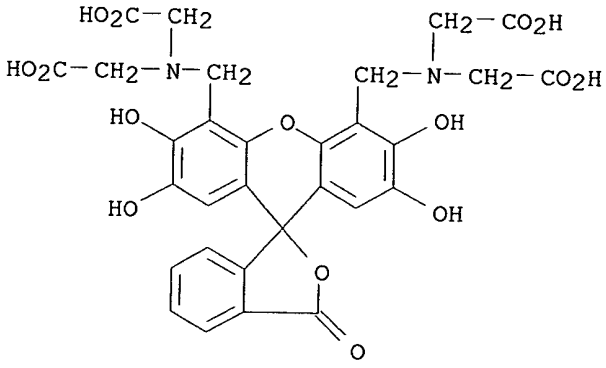


RN 5188-44-3 HCAPLUS
CN Glycine, N,N',N'',N'''-[(3',6',8'-trihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2',4',5',7'-tetrayl)tetrakis(methylene)]tetrakis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)

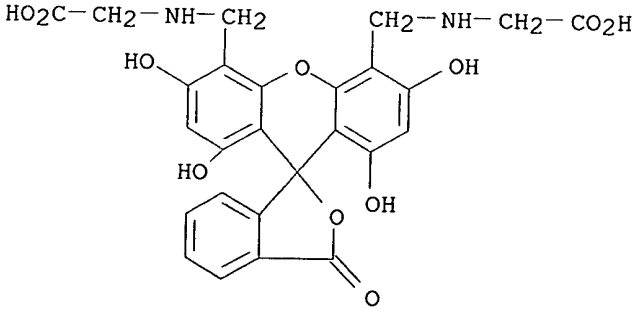




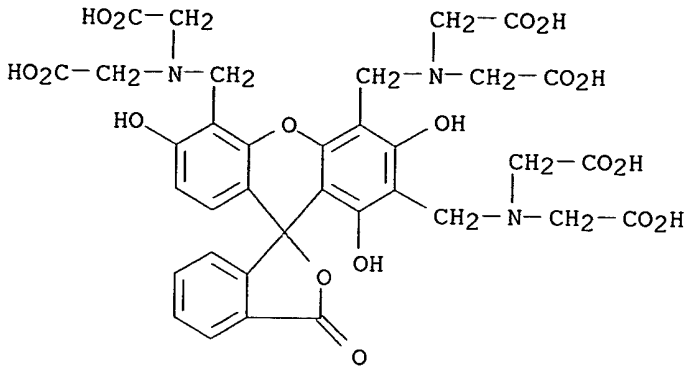
RN 5489-73-6 HCAPLUS
CN Glycine, N,N'-[(2',3',6',7'-tetrahydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4,5-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)



RN 6023-01-4 HCAPLUS
CN Glycine, N,N'-[(1',3',6',8'-tetrahydroxyfluoran-4',5'-diyl)dimethylene]di- (8CI) (CA INDEX NAME)



RN 105840-96-8 HCAPLUS
CN Fluoran, 2',4',5'-tris[[bis(carboxymethyl)amino]methyl]-1',3',6'-trihydroxy- (7CI) (CA INDEX NAME)



L61 ANSWER 21 OF 21 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1965:471846 HCAPLUS
DOCUMENT NUMBER: 63:71846
ORIGINAL REFERENCE NO.: 63:13210c-f
TITLE: Polyacetylene compounds. LXXXIII. Synthesis and determination of the absolute configuration of angelic acid ester from Aster novi-belgii.
AUTHOR(S): Bohlmann, Ferdinand; Grau, Gerhard
CORPORATE SOURCE: Tech. Univ., Berlin
SOURCE: Chem. Ber. (1965), 98(8), 2608-10
DOCUMENT TYPE: Journal
LANGUAGE: German

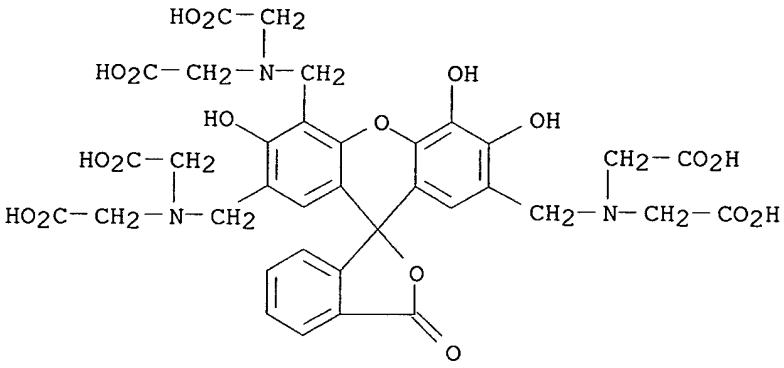
AB The abs. configuration of cis-MeCH:CMeCO2CHEt(C.tplbond.C)2CH:CHCO2Et (I) from A. novi-belgii was verified by the synthesis of the optically active trans-hydroxylachnophyllum acid from optically active EtCH(OH)C.tplbond.CH (II). The uv isomerization of the synthetic trans-ester yielded I identical with the natural product. II (1.88 g.), 225 mg. NH2OH.HCl, 222 mg. CuCl, and 1.65 g. 50% aq. EtNH2 in 50 cc. MeOH treated with stirring at 30.degree. with 3.2 g. trans-Br C.tplbond.CCH:CHCO2Me (III) in 20 cc. MeOH, and the crude product chromatographed gave 2.8 g. trans-EtCH(OH)(C.tplbond.C)2CH:CHCO2Me (IV) which, irradiated 2 hrs. with stirring in 600 cc. Et2O and chromatographed, gave 150 mg. trans,trans-EtCOCH:CHC.tplbond.CCH:CHCO2Me, m. 74.degree. (petr. ether), 1.25 g. IV, and 870 mg. oily cis isomer (V) of IV, .lambda. 305, 287, 272 m.mu.. Angelic acid (366 mg.) and 600 mg. carbodiimidazole in 5 cc. tetrahydrofuran treated 12 hrs. at 20.degree. with 351 mg. V and 20 mg. NaNH2 in 5 cc. tetrahydrofuran yielded 370 mg. oily I, .lambda. 303,285, 270 m.mu.. II (8.4 g.) in 15 cc. C5H5N and 20.2 g. m-nitrophthalic anhydride heated 3 hrs. at 80.degree. gave 79% hemiester (VI), m. 135.degree.. VI (13.57 g.) and 19.3 g. brucine in 250 cc. MeOH yielded 7.9 g. brucine salt, m. 132.degree. [.alpha.]20546 -40.8.degree. (c 2.5, MeOH), which heated in MeOH with a slight excess HCl gave 3.2 g. (-)-VI, m. 136.degree., [.alpha.]20546 -0.4.degree. (c 2.5, MeOH). (-)-VI (3.2 g.) sapond. with 2.6 g. KOH in 3 cc. H2O and 3 cc. MeOH at 20.degree. yielded 65% (+)-II, [.alpha.]20546 36.8.degree. (c 2.5, Et2O). (+)-II (163 mg.) in C5H5N with AcCl gave 200 mg. acetate, [.alpha.]20546 116.degree. (c 2.5, Et2O); a 65-mg. portion in 6.1 cc. H2O and 3 cc. Me2CO treated during 3 hrs. with cooling with 274 mg. KMnO4 in 9 cc. H2O and acidified after 3 hrs. yielded 87 mg. D(+)-EtCH(OAc)CO2H, b0.01 70-80.degree., m.

38-41.degree., [.alpha.]20D 36.2.degree. (c 3.2, MeOH); a 53-mg. portion sapond. at 20.degree. with 100 mg. NaOH in 2 cc. H2O and acidified yielded 26 mg. (+)-EtCH(OH)CO2H, m. 40-2.degree., [.alpha.]20546 3.1.degree. (c 1.3, MeOH). (+)-II (270 mg.) with III yielded 45% (+)-IV, [.alpha.]20546 13.9.degree. (c 2.3, MeOH); a 100-mg. portion sapond. with 300 mg. KOH in 0.5 cc. H2O and 2 cc. MeOH at 20.degree. yielded 80 mg. trans-EtCH(OH)(C.tplbond.C)2CH:CHCO2H, m. 97.degree. (CHCl3-CCl4), [.alpha.]20546 28.0.degree. (c 2.3, Et2O).

IT **5070-22-4**, Fluoran, 2',4',7'-tris[[bis(carboxymethyl)amino]-methyl]-3',5',6'-trihydroxy- **5119-27-7**, Fluoran, 4',5'-bis[[bis(carboxymethyl)amino]methyl]-1',3',6',8'-tetrahydroxy- **5143-11-3**, Fluoran, 4',5'-bis[[(carboxymethyl)amino]methyl]-2',3',6',7'-tetrahydroxy- **5188-44-3**, Fluoran, 2',4',5',7'-tetrakis[[bis(carboxymethyl)-amino]methyl]-1',3',6'-trihydroxy- **5489-73-6**, Fluoran, 4',5'-bis[[bis(carboxymethyl)amino]methyl]-2',3',6',7'-tetrahydroxy- **6023-01-4**, Fluoran, 4',5'-bis[[(carboxymethyl)amino]methyl]-1',3',6',8'-tetrahydroxy- **105840-96-8**, Fluoran, 2',4',5'-tris[[bis(carboxymethyl)amino]-methyl]-1',3',6'-trihydroxy-(?)
(prepn. of)

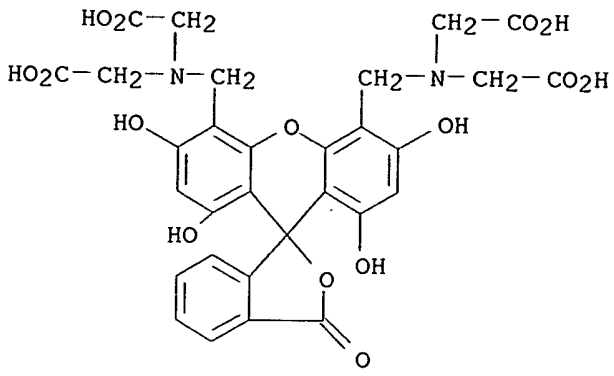
RN 5070-22-4 HCAPLUS

CN Acetic acid, [(3',5',6'-trihydroxy-3-oxospiro[phthalan-1,9'-xanthene]-2',4',7'-triyl)tris(methylenenitrilo)]hexa- (8CI) (CA INDEX NAME)

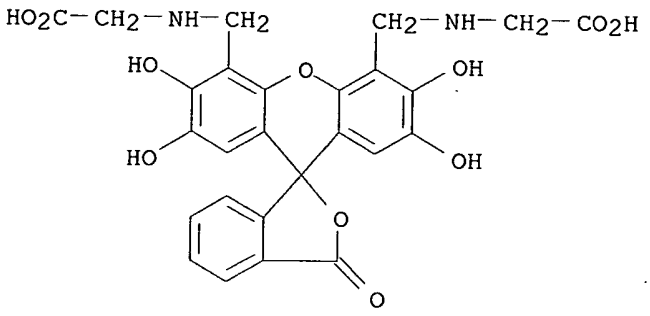


RN 5119-27-7 HCAPLUS

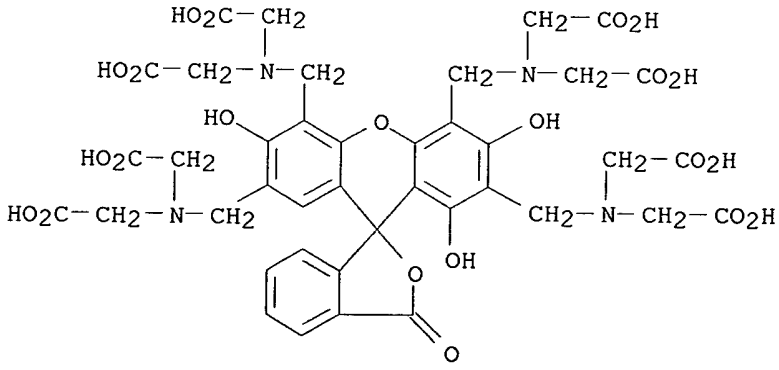
CN Acetic acid, [(1',3',6',8'-tetrahydroxyspiro[phthalan-1,9'-xanthene]-4',5'-diyl)bis(methylenenitrilo)]tetra- (8CI) (CA INDEX NAME)



RN 5143-11-3 HCAPLUS
CN Glycine, N,N'-[(2',3',6',7'-tetrahydroxyspiro[phthalan-1,9'-xanthene]-4',5'-diyl)dimethylene]di- (8CI) (CA INDEX NAME)

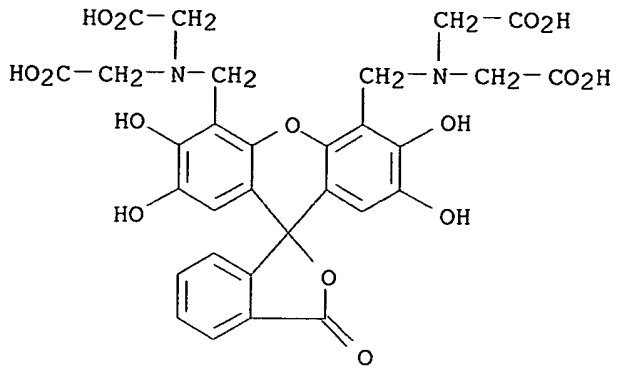


RN 5188-44-3 HCAPLUS
CN Glycine, N,N',N'',N'''-[(3',6',8'-trihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-2',4',5',7'-tetrayl)tetrakis(methylene)]tetrakis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)

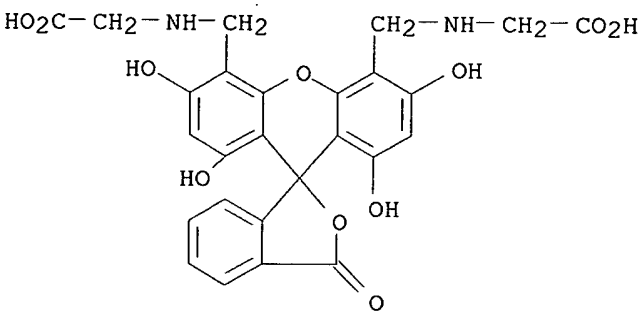


RN 5489-73-6 HCAPLUS
CN Glycine, N,N'-[(2',3',6',7'-tetrahydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-4,5-diyl)bis(methylene)]bis[N-(carboxymethyl)- (9CI) (CA

INDEX NAME)



RN 6023-01-4 HCAPLUS
CN Glycine, N,N'-[(1',3',6',8'-tetrahydroxyfluoran-4',5'-diyl)dimethylene]di- (8CI) (CA INDEX NAME)



RN 105840-96-8 HCAPLUS
CN Fluoran, 2',4',5'-tris[[bis(carboxymethyl)amino]methyl]-1',3',6'-trihydroxy- (7CI) (CA INDEX NAME)